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Complexity of numerical integration over spherical caps in a Sobolev space setting

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ABSTRACT

Let $r \geq 2$, let $\mathbb{S}^r$ be the unit sphere in $\mathbb{R}^{r+1}$, and let $\mathcal{C}(\mathbf{z};\gamma) := \{\mathbf{x} \in \mathbb{S}^r : \mathbf{x}\cdot\mathbf{z} \geq \cos\gamma\}$ be the spherical cap with center $\mathbf{z} \in \mathbb{S}^r$ and radius $\gamma \in (0,\pi]$. Let $H^s(\mathbb{S}^r)$ be the Sobolev (Hilbert) space of order s of functions on the sphere $\mathbb{S}^r$, and let Q_m be a rule for numerical integration over $\mathcal{C}(\mathbf{z};\gamma)$ with m nodes in $\mathcal{C}(\mathbf{z};\gamma)$. Then the worst-case error of the rule Q_m in $H^s(\mathbb{S}^r)$, with $s > r/2$, is bounded below by $c_{r,s,\gamma}\, m^{-s/r}$. The worst-case error in $H^s(\mathbb{S}^r)$ of any rule $Q_{m(n)}$ that has $m(n)$ nodes in $\mathcal{C}(\mathbf{z};\gamma)$, positive weights, and is exact for all spherical polynomials of degree $\leq n$ is bounded above by $\tilde{c}_{r,s,\gamma}\, n^{-s}$.

If positive weight rules $Q_{m(n)}$ with $m(n)$ nodes in $\mathcal{C}(\mathbf{z};\gamma)$ and polynomial degree of exactness n have $m(n) \sim n^r$ nodes, then the worst-case error is bounded above by $\hat{c}_{r,s,\gamma}\,(m(n))^{-s/r}$, giving the same order $m^{-s/r}$ as in the lower bound. Thus the complexity in $H^s(\mathbb{S}^r)$ of numerical integration over $\mathcal{C}(\mathbf{z};\gamma)$ with m nodes is of the order $m^{-s/r}$. The constants $c_{r,s,\gamma}$ and $\hat{c}_{r,s,\gamma}$ in the lower and upper bounds do not depend in the same way on the area $|\mathcal{C}(\mathbf{z};\gamma)| \sim \gamma^r$ of the cap. A possible explanation for this discrepancy in the behavior of the constants is given. We also explain how the lower and upper bounds on the worst-case error in a Sobolev space setting can be extended to numerical integration over a general non-empty closed and connected measurable subset Ω of $\mathbb{S}^r$ that is the closure of an open set.

1. Introduction

Numerical integration over the Euclidean unit sphere $\mathbb{S}^r \subset \mathbb{R}^{r+1}$,

$$\mathbb{S}^r := \left\{\mathbf{x} \in \mathbb{R}^{r+1} : \ \|\mathbf{x}\| = 1\right\},$$

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where $r \geq 2$ and $\|\cdot\|$ is the Euclidean norm on $\mathbb{R}^{r+1}$, has attracted much attention in the last few years (for example, see [2,3,7,17,18] and the survey [12]). Numerical integration over the sphere is needed for the discretization of integrals in some geophysical applications, such as oceanography and the modeling of the Earth's gravitational potential and magnetic field. Often the interest is not in a global problem but rather in a local one, and thus (local) rules for numerical integration over subsets of the sphere with a high polynomial degree of exactness are of great interest. In this paper we are concerned with an error analysis for numerical integration over a *(closed) spherical cap* $\mathcal{C}(\mathbf{z};\gamma)$, defined by

$$\mathcal{C}(\mathbf{z};\gamma) := \left\{\mathbf{x} \in \mathbb{S}^r : \mathbf{x}\cdot\mathbf{z} \geq \cos\gamma\right\}, \tag{1.1}$$

in a Sobolev space setting. Here $\mathbf{x}\cdot\mathbf{z}$ denotes the Euclidean inner product of $\mathbf{x}$ and $\mathbf{z}$ in $\mathbb{R}^{r+1}$.

The first paper that considers rules for numerical integration over a spherical cap with a high polynomial degree of exactness appears to be [15]. In [15], Mhaskar constructs rules for numerical integration over a closed spherical cap on $\mathbb{S}^r$ starting with a set of scattered points and selecting judiciously a subset as nodes for the numerical integration rule. In [16], Mhaskar generalizes these results to construct numerical integration rules over more general compact subsets of the sphere. The rules in [15,16] are exact for spherical polynomials of degree $\leq n$, but there is no clear indication about the relation between the number of nodes and the degree of polynomial exactness. In [5], Dai and Wang improve Mhaskar's results by showing that a point set of the exact order n^r satisfying certain conditions gives rise to a positive weight rule for numerical integration over $\mathcal{C}(\mathbf{z};\gamma) \subset \mathbb{S}^r$ that is exact for all spherical polynomials of degree $\leq n$.

In [13], Hesse and Womersley derive rules $Q_{m(n)}$ for numerical integration over $\mathcal{C}(\mathbf{z};\gamma) \subset \mathbb{S}^r$ that have $m(n)$ nodes in $\mathcal{C}(\mathbf{z};\gamma)$, have positive weights, and are exact for all (spherical) polynomials of degree $\leq n$. These rules are obtained using the standard construction of tensor product rules for product domains (see [21, Chapter 2]), and the number of nodes $m(n)$ of these rules is of the exact order n^r.

This paper considers m-point rules Q_m for *numerical integration* over the spherical cap $\mathcal{C}(\mathbf{z};\gamma)$,

$$Q_m[f] := \sum_{j=1}^{m} w_j f(\mathbf{x}_j), \tag{1.2}$$

with nodes $\mathbf{x}_j \in \mathcal{C}(\mathbf{z};\gamma)$ and weights $w_j \in \mathbb{R}$, $j = 1, 2, \ldots, m$, for approximating the *integral*

$$I_{\mathcal{C}(\mathbf{z};\gamma)}[f] := \int_{\mathcal{C}(\mathbf{z};\gamma)} f(\mathbf{x})\,\mathrm{d}\omega_r(\mathbf{x}) \tag{1.3}$$

of a continuous function f, defined on $\mathbb{S}^r$, over the spherical cap $\mathcal{C}(\mathbf{z};\gamma)$. In (1.3), $\mathrm{d}\omega_r$ denotes the usual (Lebesgue) surface element of $\mathbb{S}^r$.

The *worst-case error* $E(Q_m; H)$ of Q_m in a Hilbert space $H = H(\mathbb{S}^r)$ of continuous functions on $\mathbb{S}^r$ with norm $\|\cdot\|_H$ is defined by

$$E(Q_m; H) := \sup_{\substack{f\in H,\\ \|f\|_H\leq 1}} \left|Q_m[f] - I_{\mathcal{C}(\mathbf{z};\gamma)}[f]\right|. \tag{1.4}$$

In our analysis the Hilbert space H is the *Sobolev space* $H^s(\mathbb{S}^r)$, where $s > r/2$. For integer s, $H^s(\mathbb{S}^r)$ is the Hilbert space of those functions on $\mathbb{S}^r$ whose generalized distributional derivatives of order $\leq s$ are square-integrable over $\mathbb{S}^r$ (see Section 2.2). We prove the following results, where $|\mathcal{C}(\mathbf{z};\gamma)|$ denotes the area of the spherical cap $\mathcal{C}(\mathbf{z};\gamma)$.

Lower bound for the worst-case error: There exists a constant $c_{r,s} > 0$, depending only on r and s, such that for any rule Q_m for numerical integration over $\mathcal{C}(\mathbf{z};\gamma) \subset \mathbb{S}^r$ that has m nodes in $\mathcal{C}(\mathbf{z};\gamma)$, the worst-case error in $H^s(\mathbb{S}^r)$, $s > r/2$, has the *lower bound*

$$E\big(Q_m; H^s(\mathbb{S}^r)\big) \geq c_{r,s}|\mathcal{C}(\mathbf{z};\gamma)|^{1/2+s/r} m^{-s/r}. \tag{1.5}$$

Upper bound for the worst-case error: Consider rules $Q_{m(n)}$ for numerical integration over $\mathcal{C}(\mathbf{z};\gamma)$ with the following properties: (i) $Q_{m(n)}$ has $m(n)$ nodes that lie in $\mathcal{C}(\mathbf{z};\gamma)$ and $Q_{m(n)}$ has positive weights, and (ii) $Q_{m(n)}$ is exact for all (spherical) polynomials of degree $\le n$. Then there exists a constant $\tilde{c}_{r,s} > 0$, depending only on r and s, such that the worst-case error in $H^s(\mathbb{S}^r)$, $s > r/2$, of any rule $Q_{m(n)}$ with the properties (i) and (ii) above has the *upper bound*

$$E\big(Q_{m(n)}; H^s(\mathbb{S}^r)\big) \le \tilde{c}_{r,s}|\mathcal{C}(\mathbf{z};\gamma)|^{1/2+((r+1)/2-\lfloor(r+1)/2\rfloor-1)/(2r)} n^{-s}. \tag{1.6}$$

The estimate (1.6) holds also for sequences $\{Q_{m(n)}\}_{n\in\mathbb{N}}$ of rules $Q_{m(n)}$ that satisfy all assumptions above, apart from the positivity of the weights, and that satisfy in addition a certain regularity condition (see (3.2)). The constant $\tilde{c}_{r,s}$ then depends also on the sequence $\{Q_{m(n)}\}_{n\in\mathbb{N}}$.

Complexity result: In [13], Hesse and Womersley derived tensor product rules $Q_{m(n)}$ for numerical integration over $\mathcal{C}(\mathbf{z};\gamma)$ which satisfy assumptions (i) and (ii) for the upper bound (1.6) and for which the number $m(n)$ of nodes satisfies $c_1 n^r \le m(n) \le c_2 n^r$, with positive constants c_1 and c_2 independent of n and γ. For these rules the upper bound (1.6) yields

$$E\big(Q_{m(n)}; H^s(\mathbb{S}^r)\big) \le \tilde{c}_{r,s} c_2^{s/r} |\mathcal{C}(\mathbf{z};\gamma)|^{1/2+((r+1)/2-\lfloor(r+1)/2\rfloor-1)/(2r)} \big(m(n)\big)^{-s/r}. \tag{1.7}$$

Since the lower bound (1.5) and the upper bound (1.7) are of the same order of m, the *complexity* in $H^s(\mathbb{S}^r)$, $s > r/2$, of numerical integration over a spherical cap $\mathcal{C}(\mathbf{z};\gamma)$ with m nodes in $\mathcal{C}(\mathbf{z};\gamma)$ is of the order $m^{-s/r}$. The estimates (1.5) and (1.7) are *optimal* with respect to the order of m.

One drawback of the results is that the constants in the lower bound (1.5) and in the upper bound (1.6) do not have the same order of the area $|\mathcal{C}(\mathbf{z};\gamma)|$ of the spherical cap. It seems possible that the order of $|\mathcal{C}(\mathbf{z};\gamma)|$ in (1.5) is optimal and that the different order of $|\mathcal{C}(\mathbf{z};\gamma)|$ in the upper bounds (1.6) is partially an artifact of the method of proof and partially due to the fact that we use global (rather than local) Sobolev space norms.

For a general non-empty *closed and connected measurable subset Ω of $\mathbb{S}^r$ that is the closure of an open set*, lower and upper bounds on the worst-case error of numerical integration over Ω in a Sobolev space setting can be proved by choosing two spherical caps $\mathcal{C}(\mathbf{z}_1;\gamma_1)$ and $\mathcal{C}(\mathbf{z}_2;\gamma_2)$ such that $\mathcal{C}(\mathbf{z}_1;\gamma_1) \subset \Omega \subset \mathcal{C}(\mathbf{z}_2;\gamma_2)$ and by modifying the proofs of (1.5) and (1.6) suitably. This yields similar results to (1.5) and (1.6), which are stated in the last section of the paper.

The methods of proof were inspired by the proofs of analogous results for numerical integration over the whole sphere $\mathbb{S}^r$ in a Sobolev space setting. Lower bounds for the worst-case error of numerical integration over $\mathbb{S}^r$ in $H^s(\mathbb{S}^r)$, $s > r/2$, were derived in [9] for $r = 2$ and in [7] for general $r \ge 2$. Upper bounds for the worst-case error in $H^s(\mathbb{S}^r)$, $s > r/2$, of positive weight rules (or sequences of rules satisfying a regularity condition) that are exact for all spherical polynomials of degree $\le n$ were derived in [10] and [11] for $r = 2$ and in [2] for general $r \ge 2$.

This paper is organized as follows. In Section 2, we introduce basic background material and define the Sobolev spaces $H^s(\mathbb{S}^r)$, and in Section 3, we state the results. In Section 4, we prove the lower bounds for the worst-case error, and in Section 5 we prove the upper bounds for the worst-case error. In Section 6, we discuss the extension of the results to a general non-empty closed and connected measurable subset $\Omega \subset \mathbb{S}^r$ that is the closure of an open set.

2. Preliminaries

In Section 2.1, we introduce general notation, and in Section 2.2 we review spherical harmonics, polynomials, and Sobolev spaces on the sphere $\mathbb{S}^r$ and some of their properties.

2.1. General notation

In this paper $c, c_1, c_2, \ldots$ will denote generic positive constants that may assume different values at different places, even within the same formula. Such generic constants may depend on the sphere dimension r, the Sobolev space index s, and other parameters as indicated.

For two sequences $\{a_\ell\}_{\ell\in\mathbb{N}_0}$ and $\{b_\ell\}_{\ell\in\mathbb{N}_0}$, the notation $a_\ell \sim b_\ell$ means that there exist positive constants c_1 and c_2 such that $c_1 b_\ell \le a_\ell \le c_2 b_\ell$ for all $\ell \in \mathbb{N}_0$.

Throughout this paper, let $r \in \mathbb{N}$ satisfy $r \geq 2$. Vectors in $\mathbb{R}^{r+1}$ are denoted by boldface letters $\mathbf{x} = (x_1, x_2, \ldots, x_{r+1})^T$, and $\mathbf{x} \cdot \mathbf{y}$ denotes the Euclidean inner product of $\mathbf{x}$ and $\mathbf{y}$ in $\mathbb{R}^{r+1}$, and $\|\mathbf{x}\| = \sqrt{\mathbf{x}\cdot\mathbf{x}}$ denotes the Euclidean norm of $\mathbf{x} \in \mathbb{R}^{r+1}$.

The *unit sphere* $\mathbb{S}^r$ in $\mathbb{R}^{r+1}$ has the surface area

$$|\mathbb{S}^r| = \int_{\mathbb{S}^r} \mathrm{d}\omega_r(\mathbf{x}) = \frac{2\pi^{(r+1)/2}}{\Gamma((r+1)/2)},$$

where $\mathrm{d}\omega_r$ is the usual (Lebesgue) surface element of the sphere $\mathbb{S}^r$. By using polar coordinates with respect to $\mathbf{z}$ as the north pole and the additional substitution $t = \cos\theta_{r-1} = \mathbf{x}\cdot\mathbf{z}$ (see [7, page 418] and [4, Subsection 11.1.1]), we obtain for any integrable function $g : [-1, 1] \to \mathbb{R}$

$$\begin{aligned}\int_{\mathcal{C}(\mathbf{z};\gamma)} g(\mathbf{x}\cdot\mathbf{z})\,\mathrm{d}\omega_r(\mathbf{x}) &= \int_{\mathbb{S}^{r-1}} \int_{\cos\gamma}^{1} g(t)(1-t^2)^{(r-2)/2}\,\mathrm{d}t\,\mathrm{d}\omega_{r-1}(\mathbf{u}) \\ &= |\mathbb{S}^{r-1}| \int_{\cos\gamma}^{1} g(t)(1-t^2)^{(r-2)/2}\,\mathrm{d}t. \end{aligned} \tag{2.1}$$

Substituting in (2.1) $g \equiv 1$ and $t = \cos\theta$, $\theta \in [0, \gamma]$, the area $|\mathcal{C}(\mathbf{z};\gamma)|$ of the spherical cap $\mathcal{C}(\mathbf{z};\gamma)$, defined by (1.1), is given by

$$|\mathcal{C}(\mathbf{z};\gamma)| = \int_{\mathcal{C}(\mathbf{z};\gamma)} \mathrm{d}\omega_r(\mathbf{x}) = |\mathbb{S}^{r-1}| \int_{\cos\gamma}^{1} (1-t^2)^{(r-2)/2}\,\mathrm{d}t = |\mathbb{S}^{r-1}| \int_0^{\gamma} (\sin\theta)^{r-1}\,\mathrm{d}\theta.$$

From $|\mathcal{C}(\mathbf{z};\gamma)| \geq |\mathcal{C}(\mathbf{z};\gamma/2)|$, $2\theta/\pi \leq \sin\theta$ for all $\theta \in [0, \pi/2]$, and $\sin\theta \leq \theta$ for all $\theta \in [0, \pi]$,

$$\left(\frac{1}{\pi}\right)^{r-1} \frac{|\mathbb{S}^{r-1}|}{2r}\gamma^r \leq |\mathcal{C}(\mathbf{z};\gamma)| \leq \frac{|\mathbb{S}^{r-1}|}{r}\gamma^r \quad \text{for all } 0 \leq \gamma \leq \pi. \tag{2.2}$$

The *geodesic distance* $\mathrm{dist}(\mathbf{x}, \mathbf{y}) \in [0, \pi]$ between $\mathbf{x}$ and $\mathbf{y}$ on $\mathbb{S}^r$ is defined by

$$\mathrm{dist}(\mathbf{x}, \mathbf{y}) := \arccos(\mathbf{x}\cdot\mathbf{y}).$$

2.2. Functions on the sphere

Let $L_2(\mathbb{S}^r)$ denote the Hilbert space of (real-valued) square-integrable functions on $\mathbb{S}^r$ with the inner product

$$(f, g)_{L_2(\mathbb{S}^r)} := \int_{\mathbb{S}^r} f(\mathbf{x})g(\mathbf{x})\,\mathrm{d}\omega_r(\mathbf{x})$$

and the induced norm $\|f\|_{L_2(\mathbb{S}^r)} := (f, f)_{L_2(\mathbb{S}^r)}^{1/2}$. The space of continuous functions on $\mathbb{S}^r$ is denoted by $C(\mathbb{S}^r)$ and is endowed with the supremum norm

$$\|f\|_{C(\mathbb{S}^r)} := \sup_{\mathbf{x}\in\mathbb{S}^r} |f(\mathbf{x})|.$$

A *spherical harmonic* of degree $\ell \in \mathbb{N}_0$ (for the sphere $\mathbb{S}^r$) is the restriction of a homogeneous harmonic polynomial on $\mathbb{R}^{r+1}$ of exact degree ℓ to the unit sphere $\mathbb{S}^r$. The vector space of all spherical harmonics of degree ℓ (and the zero function) is denoted by $\mathbb{H}_\ell(\mathbb{S}^r)$ and has the dimension $Z(r,\ell) := \dim(\mathbb{H}_\ell(\mathbb{S}^r))$ given by

$$Z(r, 0) = 1 \quad \text{and} \quad Z(r,\ell) = \frac{(2\ell + r - 1)\Gamma(\ell + r - 1)}{\Gamma(\ell+1)\Gamma(r)} \quad \text{for } \ell \in \mathbb{N}.$$

From [1, 6.1.46], the asymptotic behavior of $Z(r,\ell)$ is $Z(r,\ell) \sim (\ell+1)^{r-1}$. In this paper

$$\left\{Y_{\ell,k} : k = 1, 2, \ldots, Z(r,\ell)\right\}, \tag{2.3}$$

is always a (fixed arbitrary) $L_2(\mathbb{S}^r)$-orthonormal basis of $\mathbb{H}_\ell(\mathbb{S}^r)$, consisting of real-valued spherical harmonics of degree ℓ. Any two spherical harmonics of different degree are $L_2(\mathbb{S}^r)$-orthogonal to each other, and the union of the sets (2.3) for $\ell \in \mathbb{N}_0$ forms a complete orthonormal system for $L_2(\mathbb{S}^r)$. Thus any function $f \in L_2(\mathbb{S}^r)$ can be represented in $L_2(\mathbb{S}^r)$-sense by its *Fourier series* (or Laplace series)

$$f = \sum_{\ell=0}^{\infty} \sum_{k=1}^{Z(r,\ell)} \widehat{f}_{\ell,k} Y_{\ell,k},$$

with the Fourier coefficients $\widehat{f}_{\ell,k}$ defined by

$$\widehat{f}_{\ell,k} := \big(f, Y_{\ell,k}\big)_{L_2(\mathbb{S}^r)} = \int_{\mathbb{S}^r} f(\mathbf{x}) Y_{\ell,k}(\mathbf{x})\, \mathrm{d}\omega_r(\mathbf{x}).$$

The *space* $\mathbb{P}_n(\mathbb{S}^r)$ *of spherical polynomials of degree* $\leq n$ is the set of the restrictions to $\mathbb{S}^r$ of all polynomials on $\mathbb{R}^{r+1}$ of degree $\leq n$. We have $\mathbb{P}_n(\mathbb{S}^r) = \bigoplus_{\ell=0}^{n} \mathbb{H}_\ell(\mathbb{S}^r)$ and

$$\dim\big(\mathbb{P}_n(\mathbb{S}^r)\big) = \sum_{\ell=0}^{n} Z(r,\ell) = Z(r+1,n) \sim (n+1)^r.$$

Any orthonormal basis (2.3) of $\mathbb{H}_\ell(\mathbb{S}^r)$ satisfies the *addition theorem* (see [4, Section 11.4])

$$\sum_{k=0}^{Z(r,\ell)} Y_{\ell,k}(\mathbf{x}) Y_{\ell,k}(\mathbf{y}) = \frac{Z(r,\ell)}{|\mathbb{S}^r|} P_\ell(r+1; \mathbf{x}\cdot\mathbf{y}), \quad \mathbf{x},\mathbf{y} \in \mathbb{S}^r, \tag{2.4}$$

where $P_\ell(r+1;\cdot)$ is the *normalized Legendre polynomial* of degree ℓ for $\mathbb{R}^{r+1}$, defined in terms of the Jacobi polynomial $P_\ell^{(\alpha,\beta)}$ with indices $\alpha = \beta = (r-2)/2$ via

$$P_\ell(r+1; t) := \frac{P_\ell^{((r-2)/2,(r-2)/2)}(t)}{P_\ell^{((r-2)/2,(r-2)/2)}(1)}, \quad t \in [-1,1].$$

The *Jacobi polynomials* $\{P_\ell^{(\alpha,\beta)}\}_{\ell\in\mathbb{N}_0}$ (see [22, Chapter IV]) form a complete set of orthogonal polynomials on the interval $[-1,1]$ with respect to the weighted inner product

$$(f,g)_{L_2^{(\alpha,\beta)}([-1,1])} := \int_{-1}^{1} f(t)g(t)(1-t)^\alpha(1+t)^\beta\, \mathrm{d}t.$$

The normalization is such that (see [22, (4.1.1) and (4.3.3)])

$$P_\ell^{(\alpha,\beta)}(1) = \frac{\Gamma(\ell+\alpha+1)}{\Gamma(\alpha+1)\Gamma(\ell+1)},$$
$$\int_{-1}^{1} |P_\ell^{(\alpha,\beta)}(t)|^2 (1-t)^\alpha(1+t)^\beta\, \mathrm{d}t = \frac{2^{\alpha+\beta+1}}{(2\ell+\alpha+\beta+1)} \frac{\Gamma(\ell+\alpha+1)\Gamma(\ell+\beta+1)}{\Gamma(\ell+1)\Gamma(\ell+\alpha+\beta+1)}.$$

The *Laplace–Beltrami operator* Δ^* for the unit sphere $\mathbb{S}^r$ is the angular part of the Laplace operator $\Delta = \sum_{j=1}^{r+1} \partial^2/\partial x_j^2$ for $\mathbb{R}^{r+1}$. Spherical harmonics of degree ℓ on $\mathbb{S}^r$ are eigenfunctions of $-\Delta^*$; more precisely,

$$-\Delta^* Y_\ell = \ell(\ell+r-1) Y_\ell \quad \text{for all } Y_\ell \in \mathbb{H}_\ell(\mathbb{S}^r). \tag{2.5}$$

For $s \in \mathbb{R}_0^+$, the *Sobolev space* $H^s(\mathbb{S}^r)$ is defined by (see [14, Chapter 1, Remark 7.6] and [20, Definition 6.2 and Theorem 6.3] for $r \geq 2$, and [6, Sections 5.1 and 5.2] for $r = 2$)

$$H^s(\mathbb{S}^r) := \left\{ f \in L^2(\mathbb{S}^r) : \sum_{\ell=0}^{\infty} \left(\ell + \frac{r-1}{2}\right)^{2s} \sum_{k=1}^{Z(r,\ell)} |\widehat{f}_{\ell,k}|^2 < \infty \right\}.$$

The space $H^s(\mathbb{S}^r)$ is a Hilbert space with the inner product

$$(f,g)_s := \sum_{\ell=0}^{\infty}\left(\ell+\frac{r-1}{2}\right)^{2s}\sum_{k=1}^{Z(r,\ell)}\widehat{f}_{\ell,k}\widehat{g}_{\ell,k}$$

and the induced norm

$$\|f\|_s := (f,f)_s^{1/2} = \left(\sum_{\ell=0}^{\infty}\left(\ell+\frac{r-1}{2}\right)^{2s}\sum_{k=1}^{Z(r,\ell)}|\widehat{f}_{\ell,k}|^2\right)^{1/2}. \tag{2.6}$$

If $s > r/2$, then $H^s(\mathbb{S}^r)$ is embedded into the space $C(\mathbb{S}^r)$ of continuous functions on $\mathbb{S}^r$, endowed with the supremum norm, that is, (i) $H^s(\mathbb{S}^r) \subset C(\mathbb{S}^r)$ and (ii) there exists a positive constant c such that $\|f\|_{C(\mathbb{S}^r)} \le c\|f\|_{H^s(\mathbb{S}^r)}$ for all $f \in H^s(\mathbb{S}^r)$.

For even integer s and a function $f : \mathbb{S}^r \to \mathbb{R}$ that is so smooth that the differential operator $\left[(\frac{r-1}{2})^2 - \Delta^*\right]^{s/2}$ and the summation in the Fourier series expansion of f may be interchanged, we have from (2.6), $(\ell+\frac{r-1}{2})^2 = (\frac{r-1}{2})^2 + \ell(\ell+r-1)$, and (2.5),

$$\|f\|_s = \left\|\left[\left(\frac{r-1}{2}\right)^2 - \Delta^*\right]^{s/2} f\right\|_{L_2(\mathbb{S}^r)}. \tag{2.7}$$

Furthermore, if $s > r/2$, the Sobolev space $H^s(\mathbb{S}^r)$ is a *reproducing kernel Hilbert space*. This means that there exists a uniquely determined kernel $K_s : \mathbb{S}^r \times \mathbb{S}^r \to \mathbb{R}$, the so-called reproducing kernel, with the following properties: (i) $K_s(\mathbf{x},\mathbf{y}) = K_s(\mathbf{y},\mathbf{x})$ for all $\mathbf{x},\mathbf{y} \in \mathbb{S}^r$, (ii) $K_s(\cdot,\mathbf{y}) \in H^s(\mathbb{S}^r)$ for all (fixed) $\mathbf{y} \in \mathbb{S}^r$, and (iii) the reproducing property

$$\big(f, K_s(\cdot,\mathbf{y})\big)_{H^s(\mathbb{S}^r)} = f(\mathbf{y}) \quad \text{for all } f \in H^s(\mathbb{S}^r) \text{ and all } \mathbf{y} \in \mathbb{S}^r. \tag{2.8}$$

For $H^s(\mathbb{S}^r)$ with $s > r/2$, the reproducing kernel K_s is given by

$$\begin{aligned} K_s(\mathbf{x},\mathbf{y}) &:= \sum_{\ell=0}^{\infty}\left(\ell+\frac{r-1}{2}\right)^{-2s}\sum_{k=1}^{Z(r,\ell)} Y_{\ell,k}(\mathbf{x})Y_{\ell,k}(\mathbf{y}) \\ &= \sum_{\ell=0}^{\infty}\left(\ell+\frac{r-1}{2}\right)^{-2s}\frac{Z(r,\ell)}{|\mathbb{S}^r|}P_\ell(r+1;\mathbf{x}\cdot\mathbf{y}), \end{aligned} \tag{2.9}$$

where the second representation in (2.9) follows from the addition theorem (2.4).

3. Lower and upper bounds on the worst-case error for numerical integration over a spherical cap in Sobolev spaces

We consider the approximation of the integral $I_{\mathcal{C}(\mathbf{z};\gamma)}$, defined by (1.3), for functions in the Sobolev space $H^s(\mathbb{S}^r)$ by a numerical integration rule Q_m, defined by (1.2) with m nodes $\mathbf{x}_j$ in $\mathcal{C}(\mathbf{z};\gamma)$. We measure the performance of the rule in $H^s(\mathbb{S}^r)$ by considering the *worst-case error* $E(Q_m; H^s(\mathbb{S}^r))$, defined by (1.4) with $H = H^s(\mathbb{S}^r)$. We prove the following two results.

Theorem 1. *Let $r \ge 2$ and $s > r/2$, and let $\mathcal{C}(\mathbf{z};\gamma)$ be a spherical cap on $\mathbb{S}^r$. Then there exists a positive constant $c_{r,s}$ such that the worst-case error in $H^s(\mathbb{S}^r)$ of any rule Q_m for numerical integration over $\mathcal{C}(\mathbf{z};\gamma)$, given by (1.2) with m nodes in $\mathcal{C}(\mathbf{z};\gamma)$, satisfies*

$$E\big(Q_m; H^s(\mathbb{S}^r)\big) = \sup_{\substack{f\in H^s(\mathbb{S}^r),\\ \|f\|_s\le 1}} \left|Q_m[f] - I_{\mathcal{C}(\mathbf{z};\gamma)}[f]\right| \ge c_{r,s}|\mathcal{C}(\mathbf{z};\gamma)|^{1/2+s/r}m^{-s/r}. \tag{3.1}$$

The constant $c_{r,s}$ in (3.1) depends on r and s, but not on $\mathbf{z}$, γ, Q_m, and m.

Theorem 2. *Let $r \geq 2$ and $s > r/2$, and let $\mathcal{C}(\mathbf{z};\gamma)$ be a spherical cap on $\mathbb{S}^r$. Consider a sequence $\{Q_{m(n)}\}_{n\in\mathbb{N}}$ of rules $Q_{m(n)}$ for numerical integration over $\mathcal{C}(\mathbf{z};\gamma)$ with the following properties:*

(i) *$Q_{m(n)}$ is of the form (1.2) with $m = m(n)$ nodes located in $\mathcal{C}(\mathbf{z};\gamma)$.*

(ii) *The rule $Q_{m(n)}$ is exact for all spherical polynomials of degree $\leq n$, that is,*

$$Q_{m(n)}[p] = I_{\mathcal{C}(\mathbf{z};\gamma)}[p] \quad \text{for all } p \in \mathbb{P}_n(\mathbb{S}^r).$$

(iii) *There exists a positive constant C such that, for every $Q_{m(n)}$, the weights w_j and nodes $\mathbf{x}_j$ of $Q_{m(n)}$ satisfy the* regularity condition

$$\sum_{\substack{j=1,\\ \mathbf{x}_j\in\mathcal{C}(\mathbf{y};\gamma/(\pi n))}}^{m(n)} |w_j| \leq C\left(\frac{\gamma}{\pi n}\right)^r \quad \text{for all } \mathbf{y}\in\mathbb{S}^r. \tag{3.2}$$

Then the worst-case error of $Q_{m(n)}$ in $H^s(\mathbb{S}^r)$ satisfies the estimate

$$\begin{aligned} E\big(Q_{m(n)};H^s(\mathbb{S}^r)\big) &= \sup_{\substack{f\in H^s(\mathbb{S}^r),\\ \|f\|_s\leq 1}} \big|Q_{m(n)}[f] - I_{\mathcal{C}(\mathbf{z};\gamma)}[f]\big| \\ &\leq \tilde{c}_{r,s}|\mathcal{C}(\mathbf{z};\gamma)|^{1/2+((r+1)/2-\lfloor (r+1)/2\rfloor-1)/(2r)} n^{-s}, \end{aligned} \tag{3.3}$$

where the positive constant $\tilde{c}_{r,s}$ depends on r, s, and the constant C in (3.2), but not on $\mathbf{z}$, γ, $Q_{m(n)}$, $m = m(n)$, and n.

In [13, Theorem 6.1] it was shown that there exists a positive constant C, depending only on r, such that for any rule (1.2) for numerical integration over $\mathcal{C}(\mathbf{z};\gamma)$ that has nodes $\mathbf{x}_j \in \mathcal{C}(\mathbf{z};\gamma)$, positive weights w_j, and is exact on $\mathbb{P}_n(\mathbb{S}^r)$, with $n \geq 2$, (3.2) is automatically satisfied. For such positive weight rules the constant C in (3.2) is universal. Thus we obtain the following corollary.

Corollary 3. *Let $r \geq 2$ and $s > r/2$, and let $\mathcal{C}(\mathbf{z};\gamma)$ be a spherical cap on $\mathbb{S}^r$. There exists a positive constant $\tilde{c}_{r,s}$ (depending only on r and s) such that for every rule $Q_{m(n)}$ for numerical integration over $\mathcal{C}(\mathbf{z};\gamma)$ that has $m(n)$ nodes in $\mathcal{C}(\mathbf{z};\gamma)$, positive weights, and is exact on $\mathbb{P}_n(\mathbb{S}^r)$, where $n \geq 2$, the worst-case error satisfies the estimate*

$$E\big(Q_{m(n)};H^s(\mathbb{S}^r)\big) \leq \tilde{c}_{r,s}|\mathcal{C}(\mathbf{z};\gamma)|^{1/2+((r+1)/2-\lfloor (r+1)/2\rfloor-1)/(2r)} n^{-s}. \tag{3.4}$$

It should be noted that the constant $\tilde{c}_{r,s}$ in (3.4) is *universal* for all caps $\mathcal{C}(\mathbf{z};\gamma)$, $\mathbf{z}\in\mathbb{S}^r$, $\gamma\in(0,\pi]$.

Complexity result: In [13], Hesse and Womersley derive for $n \in \mathbb{N}_0$ tensor product rules $Q_{m(n)}$ for numerical integration over the spherical cap $\mathcal{C}(\mathbf{z};\gamma)$ that have $m(n)$ nodes in $\mathcal{C}(\mathbf{z};\gamma)$, positive weights, are exact on $\mathbb{P}_n(\mathbb{S}^r)$, and satisfy $c_1 n^r \leq m(n) \leq c_2 n^r$. For such rules (3.4) implies

$$E\big(Q_{m(n)};H^s(\mathbb{S}^r)\big) \leq \tilde{c}_{r,s}c_2^{s/r}|\mathcal{C}(\mathbf{z};\gamma)|^{1/2+((r+1)/2-\lfloor (r+1)/2\rfloor-1)/(2r)} \big(m(n)\big)^{-s/r}. \tag{3.5}$$

Since the order $(m(n))^{-s/r}$ in (3.5) is the same as in (3.1), we have established that the complexity in $H^s(\mathbb{S}^r)$ of numerical integration over a spherical cap $\mathcal{C}(\mathbf{z};\gamma)$ with m nodes in the cap is of the order $m^{-s/r}$. Both the estimates (3.5) and (3.1) are optimal with respect to the order of m.

Dependence of the bounds on the area of the cap: A drawback of the results in Theorems 1 and 2 is that the bounds do not depend in the same way on the area $|\mathcal{C}(\mathbf{z};\gamma)| \sim \gamma^r$ of the cap. It seems possible that the lower bound has the correct dependence on the area $|\mathcal{C}(\mathbf{z};\gamma)|$ of the cap, whereas in the upper bound we have an additional negative power $((r+1)/2-\lfloor (r+1)/2\rfloor-1)/(2r)$ (which equals $-1/(4r)$ for even r and $-1/(2r)$ for odd r) and we lose a power s/r. It seems likely that the additional negative power $((r+1)/2-\lfloor (r+1)/2\rfloor-1)/(2r)$ is an artifact from the method of proof, whereas the missing power s/r is possibly due to the fact that global Sobolev spaces $H^s(\mathbb{S}^r)$ are used (instead of local Sobolev spaces), because the global Sobolev space norms do not change when the (size of the) cap changes. It is not immediately clear how bounds with the same dependence on the area of the cap can be achieved in the lower bound and the upper bound, even if local Sobolev spaces are used.

4. Proof of the lower bound

For the proof of Theorem 1 we need two lemmas.

Lemma 4. *Let $r \geq 2$, let $0 < \gamma \leq \pi$, and let $\mathbf{z} \in \mathbb{S}^r$ be arbitrary. For any $m \in \mathbb{N}$, there exist $M_m \geq 2m$ points $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_{M_m}$ in $\mathcal{C}(\mathbf{z}; \gamma)$ and a radius $\alpha_m \in (0, \gamma/2]$, with*

$$\alpha_m = C_{r,\gamma}(2m)^{-1/r}, \tag{4.1}$$

$$2m \leq M_m \leq 6(3\pi)^{r-1} 2m, \tag{4.2}$$

such that the caps $\mathcal{C}(\mathbf{y}_i; \alpha_m)$, $i = 1, 2, \ldots, M_m$, form a packing of $\mathcal{C}(\mathbf{z}; \gamma)$, that is, $\mathcal{C}(\mathbf{y}_i; \alpha_m)$ and $\mathcal{C}(\mathbf{y}_j; \alpha_m)$ with $i \neq j$ touch at most at the boundary and all $\mathcal{C}(\mathbf{y}_i; \alpha_m)$, $i = 1, 2, \ldots, M_m$, lie in $\mathcal{C}(\mathbf{z}; \gamma)$. The constant $C_{r,\gamma}$ in (4.1) is explicitly given by

$$C_{r,\gamma} := \frac{1}{3} \left(\frac{r|\mathcal{C}(\mathbf{z}; \gamma)|}{|\mathbb{S}^{r-1}|} \right)^{1/r}. \tag{4.3}$$

Lemma 4 is the local equivalent to [7, Lemma 1] and will be proved at the end of this section. From (2.2), clearly $C_{r,\gamma} \sim c_r \gamma$ with a positive constant c_r that depends only on r.

[7, Lemma 2] provides an interpolation result for Sobolev space norms.

Lemma 5 ([7, Lemma 2]). *Let $r \geq 2$. Consider $s \geq 0$ and choose an integer $q \in \mathbb{N}_0$ such that $2q \leq s \leq 2(q+1)$. Then for $f \in H^{2(q+1)}(\mathbb{S}^r)$*

$$\|f\|_s \leq \|f\|_{2q}^{(2q+2-s)/2} \|f\|_{2(q+1)}^{(s-2q)/2}. \tag{4.4}$$

The proof of Theorem 1 follows the proof of [7, Theorem 1] with some modifications. The idea is to construct for each m and each rule Q_m a 'bad function' $f_m \in H^s(\mathbb{S}^r)$ such that

$$\mathrm{Error}\big(Q_m[f_m/\|f_m\|_s]\big) := \frac{1}{\|f_m\|_s} \big| Q_m[f_m] - I_{\mathcal{C}(\mathbf{z};\gamma)}[f_m] \big| \geq c_{r,s} |\mathcal{C}(\mathbf{z}; \gamma)|^{1/2+s/r} m^{-s/r}. \tag{4.5}$$

Since the error for the individual function $f_m/\|f_m\|_s$ is a lower bound for the worst-case error in $H^s(\mathbb{S}^r)$, the estimate (4.5) implies then the lower bound (3.1) on the worst-case error.

Proof of Theorem 1. Due to Lemma 4, there exists a packing of the spherical cap $\mathcal{C}(\mathbf{z}; \gamma)$ with $M_m \geq 2m$ caps $\mathcal{C}(\mathbf{y}_i; \alpha_m)$, $i = 1, 2, \ldots, M_m$, where $\alpha_m = C_{r,\gamma}(2m)^{-1/r}$ with the constant $C_{r,\gamma} > 0$ given by (4.3). Since there are at least $2m$ spherical caps $\mathcal{C}(\mathbf{y}_i; \alpha_m)$, $i = 1, 2, \ldots, M_m$, but only m nodes of the numerical integration rule Q_m and since the interiors of the spherical caps $\mathcal{C}(\mathbf{y}_i; \alpha_m)$, $i = 1, 2, \ldots, M_m$, are disjoint, at most m of the spherical caps $\mathcal{C}(\mathbf{y}_i; \alpha_m)$, $i = 1, 2, \ldots, M_m$, contain a node $\mathbf{x}_j$ of the rule Q_m in the interior. Thus at least m of the spherical caps $\mathcal{C}(\mathbf{y}_i; \alpha_m)$, $i = 1, 2, \ldots, M_m$, contain no nodes $\mathbf{x}_j$ of the rule Q_m in the interior. After renumbering, we may assume that $\mathcal{C}(\mathbf{y}_i; \alpha_m)$, $i = 1, 2, \ldots, m$, contain no nodes $\mathbf{x}_j$ of the rule Q_m in the interior.

Now choose a real-valued function $\Phi \in C^\infty((-\infty, 1])$ with the following three properties: (i) $\Phi(t) = 0$ for all $t \leq 0$, (ii) $0 \leq \Phi(t) \leq 1$ for all $t \in (-\infty, 1]$, and (iii) $\Phi(t) = 1$ for all $t \in [1/2, 1]$. Clearly Φ has compact support contained in the interval $[0, 1]$. For example, we could choose the function Φ as in [8, page 543]. It is crucial to use the same function Φ (with the properties above) in the proof for all m, all rules Q_m, and all spherical caps $\mathcal{C}(\mathbf{z}; \gamma)$. The 'scaled' function

$$\Phi_m(t) := \Phi\left(\frac{t - \cos\alpha_m}{1 - \cos\alpha_m} \right), \quad t \in (-\infty, 1],$$

has then compact support contained in $[\cos\alpha_m, 1]$, and Φ_m has the value $\Phi_m(t) = 1$ if

$$\frac{1}{2} \leq \frac{t - \cos\alpha_m}{1 - \cos\alpha_m} \leq 1 \Leftrightarrow \frac{1}{2}(1 + \cos\alpha_m) = \left(\cos\frac{\alpha_m}{2}\right)^2 \leq t \leq 1.$$

Since $\alpha_m/2 \le \gamma/4 \le \pi/4$ (as we have at least two caps $\mathcal{C}(\mathbf{y}_i;\alpha_m)$), $[\cos(\alpha_m/2)]^2 \le \cos(\alpha_m/2)$, and thus

$$\Phi_m(t) = 1 \quad \text{for all } t \in \left[\cos\frac{\alpha_m}{2}, 1\right]. \tag{4.6}$$

We define our 'bad function' by

$$f_m(\mathbf{x}) := \sum_{i=1}^{m} \Phi_m(\mathbf{x}\cdot\mathbf{y}_i) = \sum_{i=1}^{m} \Phi\left(\frac{\mathbf{x}\cdot\mathbf{y}_i - \cos\alpha_m}{1-\cos\alpha_m}\right), \quad \mathbf{x}\in\mathbb{S}^r. \tag{4.7}$$

By construction, the local support of the function f_m is contained in the union of the spherical caps $\mathcal{C}(\mathbf{y}_i;\alpha_m)$, $i = 1, 2, \ldots, m$. Since there are no nodes of the rule Q_m in the interior of the support of f_m, we have $Q_m[f_m] = 0$. Thus (using also the fact that $f_m(t) \ge 0$ for all t)

$$\mathrm{Error}\big(Q_m[f_m/\|f_m\|_s]\big) = \|f_m\|_s^{-1}\big|Q_m[f_m] - I_{\mathcal{C}(\mathbf{z};\gamma)}[f_m]\big| = \|f_m\|_s^{-1} I_{\mathcal{C}(\mathbf{z};\gamma)}[f_m]. \tag{4.8}$$

Since $\Phi_m(\mathbf{x}\cdot\mathbf{y}_i)$ has local support contained in $\mathcal{C}(\mathbf{y}_i;\alpha_m)$, using (4.7), $\Phi_m(t) \ge 0$ for all $t\in\mathbb{R}$, and $\Phi_m(\mathbf{x}\cdot\mathbf{y}_i)|_{\mathbf{x}\in\mathcal{C}(\mathbf{y}_i;\alpha_m/2)} = 1$ (from (4.6)),

$$\begin{aligned}
I_{\mathcal{C}(\mathbf{z};\gamma)}[f_m] &= \sum_{i=1}^{m}\int_{\mathcal{C}(\mathbf{y}_i;\alpha_m)} \Phi_m(\mathbf{x}\cdot\mathbf{y}_i)\,\mathrm{d}\omega_r(\mathbf{x}) \ge \sum_{i=1}^{m}\int_{\mathcal{C}(\mathbf{y}_i;\alpha_m/2)} 1\,\mathrm{d}\omega_r(\mathbf{x})\\
&= m|\mathcal{C}(\mathbf{y}_1;\alpha_m/2)| \ge m\left(\frac{1}{\pi}\right)^{r-1}\frac{|\mathbb{S}^{r-1}|}{2r}\left(\frac{\alpha_m}{2}\right)^r\\
&= \frac{|\mathbb{S}^{r-1}|}{2^{r+2}\pi^{r-1}r}C_{r,\gamma}^r = \frac{|\mathcal{C}(\mathbf{z};\gamma)|}{2^{r+2}3^r\pi^{r-1}}.
\end{aligned} \tag{4.9}$$

In the last line, we have used (2.2), $\alpha_m = C_{r,\gamma}(2m)^{-1/r}$ and (4.3). Thus from (4.8) and (4.9),

$$\mathrm{Error}\big(Q_m[f_m/\|f_m\|_s]\big) \ge \frac{|\mathcal{C}(\mathbf{z};\gamma)|}{2^{r+2}3^r\pi^{r-1}}\|f_m\|_s^{-1}. \tag{4.10}$$

The proof will be complete if we can show that

$$\|f_m\|_s \le c_{r,s}|\mathcal{C}(\mathbf{z};\gamma)|^{1/2-s/r}m^{s/r}, \tag{4.11}$$

with a positive constant $c_{r,s}$ that depends only on r and s. Then from (4.11) and (4.10),

$$E\big(Q_m; H^s(\mathbb{S}^r)\big) \ge \mathrm{Error}\big(Q_m[f_m/\|f_m\|_s]\big) \ge \big(2^{r+2}3^r\pi^{r-1}c_{r,s}\big)^{-1}|\mathcal{C}(\mathbf{z};\gamma)|^{1/2+s/r}m^{-s/r}.$$

It remains to show (4.11). We do this by first proving (4.11) for s that is an even integer and then use Lemma 5 to interpolate between the even integer cases.

Consider s that is a positive even integer. Since f_m is infinitely often differentiable, we may apply the representation (2.7) of the norm $\|\cdot\|_s$. Thus, using the definition (4.7) of f_m,

$$\begin{aligned}
\|f_m\|_s^2 &= \int_{\mathbb{S}^r}\left(\sum_{i=1}^{m}\left[\left(\frac{r-1}{2}\right)^2 - \Delta^*\right]^{s/2}\Phi_m(\mathbf{x}\cdot\mathbf{y}_i)\right)^2\mathrm{d}\omega_r(\mathbf{x})\\
&= \sum_{i=1}^{m}\int_{\mathcal{C}(\mathbf{y}_i;\alpha_m)}\left|\left[\left(\frac{r-1}{2}\right)^2 - \Delta^*\right]^{s/2}\Phi_m(\mathbf{x}\cdot\mathbf{y}_i)\right|^2\mathrm{d}\omega_r(\mathbf{x}),
\end{aligned} \tag{4.12}$$

where the last equality follows from the fact that $\left[(\frac{r-1}{2})^2 - \Delta^*\right]^{s/2}\Phi_m(\mathbf{x}\cdot\mathbf{y}_i)$ has local support contained in the cap $\mathcal{C}(\mathbf{y}_i;\alpha_m)$ and the fact that the caps $\mathcal{C}(\mathbf{y}_i;\alpha_m)$, $i = 1, 2, \ldots, m$, have at most boundary points in common.

For $s = 0$, we have from $0 \le \Phi_m(t) \le 1$ for all $t \in (-\infty, 1]$, $\alpha_m = C_{r,\gamma}(2m)^{-1/r}$, and (2.2),

$$\int_{\mathcal{C}(\mathbf{y}_i;\alpha_m)} |\Phi_m(\mathbf{x}\cdot\mathbf{y}_i)|^2 \, \mathrm{d}\omega_r(\mathbf{x}) \le \int_{\mathcal{C}(\mathbf{y}_i;\alpha_m)} 1 \, \mathrm{d}\omega_r(\mathbf{x}) = |\mathcal{C}(\mathbf{y}_i;\alpha_m)| \le \frac{|\mathbb{S}^{r-1}|}{r} \frac{C_{r,\gamma}^r}{2m}. \tag{4.13}$$

Thus (4.12) and (4.13), and the definition (4.3) of $C_{r,\gamma}$ imply (4.11) for $s = 0$, as

$$\begin{aligned} \|f_m\|_0 &\le \left(\sum_{i=1}^m \frac{|\mathbb{S}^{r-1}|}{r} \frac{C_{r,\gamma}^r}{2m} \right)^{1/2} = \left(\frac{C_{r,\gamma}^r |\mathbb{S}^{r-1}|}{2r} \right)^{1/2} \\ &= \left(\frac{|\mathcal{C}(\mathbf{z};\gamma)|}{3^r 2} \right)^{1/2} = \frac{|\mathcal{C}(\mathbf{z};\gamma)|^{1/2-0/r}}{3^{r/2} 2^{1/2}} m^{0/r}. \end{aligned} \tag{4.14}$$

For $s > 0$ that is an even integer, we now parameterize each of the integrals in the last line of (4.12) with respect to the point $\mathbf{y}_i$ as the north pole: letting $t = \cos(\mathbf{x}\cdot\mathbf{y}_i)$ we find (see (2.1), and see [7, pages 418–419 and 430] and [4, Section 11.1] for the parameterization of Δ^*)

$$\begin{aligned} &\int_{\mathcal{C}(\mathbf{y}_i;\alpha_m)} \left| \left[\left(\frac{r-1}{2}\right)^2 - \Delta^* \right]^{s/2} \Phi_m(\mathbf{x}\cdot\mathbf{y}_i) \right|^2 \mathrm{d}\omega_r(\mathbf{x}) \\ &= |\mathbb{S}^{r-1}| \int_{\cos\alpha_m}^1 \left| \left[\left(\frac{r-1}{2}\right)^2 + rt\frac{\mathrm{d}}{\mathrm{d}t} - (1-t^2)\frac{\mathrm{d}^2}{\mathrm{d}t^2} \right]^{s/2} \Phi_m(t) \right|^2 (1-t^2)^{(r-2)/2} \, \mathrm{d}t \\ &\le |\mathbb{S}^{r-1}| (\sin\alpha_m)^{r-2} \int_{\cos\alpha_m}^1 \left| \left[\left(\frac{r-1}{2}\right)^2 + rt\frac{\mathrm{d}}{\mathrm{d}t} - (1-t^2)\frac{\mathrm{d}^2}{\mathrm{d}t^2} \right]^{s/2} \Phi_m(t) \right|^2 \mathrm{d}t, \end{aligned} \tag{4.15}$$

where the last line follows from $1 - t^2 \le 1 - (\cos\alpha_m)^2 = (\sin\alpha_m)^2$ for all $t \in [\cos\alpha_m, 1]$. The integrand in (4.15) can be estimated analogously to [7, pages 430–432], which yields

$$\left| \left[\left(\frac{r-1}{2}\right)^2 + rt\frac{\mathrm{d}}{\mathrm{d}t} - (1-t^2)\frac{\mathrm{d}^2}{\mathrm{d}t^2} \right]^{s/2} \Phi_m(t) \right| \le c \left(\sin\frac{\alpha_m}{2} \right)^{-s} \quad \text{for all } t \in [\cos\alpha_m, 1], \tag{4.16}$$

where the constant c depends only on r and s (and the initial choice of Φ). Substituting (4.16) into (4.15) yields (using $1 - \cos\alpha_m = 2[\sin(\alpha_m/2)]^2$)

$$\begin{aligned} &\int_{\mathcal{C}(\mathbf{y}_i;\alpha_m)} \left| \left[\left(\frac{r-1}{2}\right)^2 - \Delta^* \right]^{s/2} \Phi_m(\mathbf{x}\cdot\mathbf{y}_i) \right|^2 \mathrm{d}\omega_r(\mathbf{x}) \\ &\le |\mathbb{S}^{r-1}| (\sin\alpha_m)^{r-2} \int_{\cos\alpha_m}^1 c^2 \left(\sin\frac{\alpha_m}{2} \right)^{-2s} \mathrm{d}t \\ &= 2c^2 |\mathbb{S}^{r-1}| (\sin\alpha_m)^{r-2} \left(\sin\frac{\alpha_m}{2} \right)^{2-2s}. \end{aligned} \tag{4.17}$$

Finally, with $|\sin\alpha_m| \le |\alpha_m|$, $|\sin(\alpha_m/2)| \ge \alpha_m/\pi$, $\alpha_m = C_{r,\gamma}(2m)^{-1/r}$, and (4.3), the estimate (4.17) implies

$$\int_{\mathcal{C}(\mathbf{y}_i;\alpha_m)} \left| \left[\left(\frac{r-1}{2}\right)^2 - \Delta^* \right]^{s/2} \Phi_m(\mathbf{x}\cdot\mathbf{y}_i) \right|^2 \mathrm{d}\omega_r(\mathbf{x}) \le 2c^2 |\mathbb{S}^{r-1}| \alpha_m^{r-2} \left(\frac{\alpha_m}{\pi} \right)^{2-2s}$$

$$= c^2 2^{2s/r} \pi^{2s-2} |\mathbb{S}^{r-1}| C_{r,\gamma}^{r-2s} m^{-1+2s/r} = \frac{c^2 2^{2s/r} \pi^{2s-2} |\mathbb{S}^{r-1}|^{2s/r}}{3^{r-2s} r^{2s/r-1}} |\mathcal{C}(\mathbf{z};\gamma)|^{1-2s/r} m^{-1+2s/r}. \quad (4.18)$$

Substituting (4.18) into (4.12) yields, for s that is a positive even integer,

$$\|f_m\|_s^2 \leq \sum_{i=1}^{m} c_{r,s} |\mathcal{C}(\mathbf{z};\gamma)|^{1-2s/r} m^{-1+2s/r} = c_{r,s} |\mathcal{C}(\mathbf{z};\gamma)|^{1-2s/r} m^{2s/r}, \quad (4.19)$$

where the constant $c_{r,s}$ depends only on r and s.

The estimates (4.14) and (4.19) verify (4.11) for s that is a non-negative even integer.

For $s \geq 0$ which is not an even integer, we choose the integer $q \in \mathbb{N}_0$ such that $2q < s < 2(q+1)$. Then from (4.4) in Lemma 5 and from applying (4.11) for $\|f_m\|_{2q}$ and $\|f_m\|_{2(q+1)}$ we find

$$\begin{aligned} \|f_m\|_s &\leq \|f_m\|_{2q}^{(2q+2-s)/2} \|f_m\|_{2(q+1)}^{(s-2q)/2} \\ &\leq c_{r,2q}^{(2q+2-s)/2} c_{r,2(q+1)}^{(s-2q)/2} |\mathcal{C}(\mathbf{z};\gamma)|^{1/2-s/r} m^{s/r}, \end{aligned}$$

which proves (4.11) for all $s \geq 0$. This concludes the proof. $\square$

Proof of Lemma 4. Let α_m be of the form $\alpha_m = C_{r,\gamma}(2m)^{-1/r}$ with a constant $C_{r,\gamma}$ that will be determined later. Consider points $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_{M_m} \in \mathcal{C}(\mathbf{z};\gamma)$, where $M_m \geq 2$, such that $\{\mathcal{C}(\mathbf{y}_i;\alpha_m)\}_{i=1,2,\ldots,M_m}$ forms a *maximal* packing of $\mathcal{C}(\mathbf{z};\gamma)$. (A packing $\{\mathcal{C}(\mathbf{y}_i;\alpha_m)\}_{i=1,2,\ldots,M_m}$ is called maximal, if it is not possible to add any other cap of radius α_m to the packing.) Then the union of the areas of $\mathcal{C}(\mathbf{y}_i;\alpha_m)$, $i = 1, 2, \ldots, M_m$, is less than the area of $\mathcal{C}(\mathbf{z};\gamma)$. In formulas,

$$\sum_{i=1}^{M_m} |\mathcal{C}(\mathbf{y}_i;\alpha_m)| = M_m |\mathcal{C}(\mathbf{y}_1;\alpha_m)| \leq |\mathcal{C}(\mathbf{z};\gamma)|. \quad (4.20)$$

The lower bound from (2.2) and $\alpha_m = C_{r,\gamma}(2m)^{-1/r}$ yield in (4.20)

$$M_m \leq \frac{|\mathcal{C}(\mathbf{z};\gamma)|}{|\mathcal{C}(\mathbf{y}_1;\alpha_m)|} \leq \frac{2r|\mathcal{C}(\mathbf{z};\gamma)|}{|\mathbb{S}^{r-1}|} \pi^{r-1} \alpha_m^{-r} \leq \frac{2r|\mathcal{C}(\mathbf{z};\gamma)|}{|\mathbb{S}^{r-1}|} \pi^{r-1} C_{r,\gamma}^{-r} 2m. \quad (4.21)$$

We claim that $\{\mathcal{C}(\mathbf{y}_i;\beta_m)\}_{i=1,2,\ldots,M_m}$, where $\beta_m := \min\{3\alpha_m, \pi\}$, is a covering of $\mathcal{C}(\mathbf{z};\gamma)$, that is,

$$\mathcal{C}(\mathbf{z};\gamma) \subset \bigcup_{i=1}^{M_m} \mathcal{C}(\mathbf{y}_i;\beta_m). \quad (4.22)$$

Then (4.22) implies

$$|\mathcal{C}(\mathbf{z};\gamma)| \leq \sum_{i=1}^{M_m} |\mathcal{C}(\mathbf{y}_i;\beta_m)| = M_m |\mathcal{C}(\mathbf{y}_1;\beta_m)|. \quad (4.23)$$

Using the upper bound from (2.2) and $\beta_m \leq 3\alpha_m = 3C_{r,\gamma}(2m)^{-1/r}$, (4.23) yields

$$M_m \geq \frac{|\mathcal{C}(\mathbf{z};\gamma)|}{|\mathcal{C}(\mathbf{y}_1;\beta_m)|} \geq \frac{r|\mathcal{C}(\mathbf{z};\gamma)|}{|\mathbb{S}^{r-1}|} \beta_m^{-r} \geq \frac{r|\mathcal{C}(\mathbf{z};\gamma)|}{3^r|\mathbb{S}^{r-1}|} C_{r,\gamma}^{-r} 2m. \quad (4.24)$$

If the constant $C_{r,\gamma}$ is given by (4.3), then from (4.24) and (4.21),

$$2m \leq M_m \leq 6(3\pi)^{r-1} 2m,$$

which verifies (4.2).

It remains to show (4.22). Instead we show that $\{\mathcal{C}(\mathbf{y}_i;2\alpha_m)\}_{i=1,2,\ldots,M_m}$ forms a covering of $\mathcal{C}(\mathbf{z};\gamma-\alpha_m)$. This immediately implies (4.22): Indeed, consider an arbitrary $\mathbf{u} \in \mathcal{C}(\mathbf{z};\gamma)$. Then there exists a point $\mathbf{w} \in \mathcal{C}(\mathbf{z}; \gamma - \alpha_m)$ with $\operatorname{dist}(\mathbf{u}, \mathbf{w}) \leq \alpha_m$, and there exists a point $\mathbf{y}_k$ with $\mathbf{w} \in \mathcal{C}(\mathbf{y}_k; 2\alpha_m)$, because $\{\mathcal{C}(\mathbf{y}_i; 2\alpha_m)\}_{i=1,2,\ldots,M_m}$ forms a covering of $\mathcal{C}(\mathbf{z}; \gamma - \alpha_m)$. Thus

$$\operatorname{dist}(\mathbf{u}, \mathbf{y}_k) \leq \operatorname{dist}(\mathbf{u}, \mathbf{w}) + \operatorname{dist}(\mathbf{w}, \mathbf{y}_k) \leq \alpha_m + 2\alpha_m = 3\alpha_m.$$

Since trivially $\operatorname{dist}(\mathbf{u}, \mathbf{y}_k) \leq \pi$, we find $\operatorname{dist}(\mathbf{u}, \mathbf{y}_k) \leq \min\{3\alpha_m, \pi\} = \beta_m$, and $\mathbf{u}$ belongs to $\mathcal{C}(\mathbf{y}_k; \beta_m)$. Since $\mathbf{u} \in \mathcal{C}(\mathbf{z}; \gamma)$ was arbitrary, we see that (4.22) holds true.

Now we show that $\{\mathcal{C}(\mathbf{y}_i; 2\alpha_m)\}_{i=1,2,\ldots,M_m}$ forms a covering of $\mathcal{C}(\mathbf{z}; \gamma - \alpha_m)$. Assume that this is wrong, that is, assume that there is a point $\mathbf{u} \in \mathcal{C}(\mathbf{z}; \gamma - \alpha_m)$ that is not contained in $\bigcup_{i=1}^{M_m} \mathcal{C}(\mathbf{y}_i; 2\alpha_m)$. Then $\operatorname{dist}(\mathbf{u}, \mathbf{y}_i) > 2\alpha_m$ for all $i = 1, 2, \ldots, M_m$, and thus the caps $\mathcal{C}(\mathbf{y}_i; \alpha_m)$, $i = 1, 2, \ldots, M_m$, and $\mathcal{C}(\mathbf{u}; \alpha_m)$, touch at most at the boundary. Since $\mathbf{u} \in \mathcal{C}(\mathbf{z}; \gamma - \alpha_m)$, the cap $\mathcal{C}(\mathbf{u}; \alpha_m)$ is contained in $\mathcal{C}(\mathbf{z}; \gamma)$, and hence $\{\mathcal{C}(\mathbf{y}_i; \alpha_m)\}_{i=1,2,\ldots,M_m} \cup \{\mathcal{C}(\mathbf{u}; \alpha_m)\}$ is a packing of $\mathcal{C}(\mathbf{z}; \gamma)$. This is a contradiction to the fact that the packing $\{\mathcal{C}(\mathbf{y}_i; \alpha_m)\}_{i=1,2,\ldots,M_m}$ was maximal. Thus the assumption was wrong, and $\{\mathcal{C}(\mathbf{y}_i; 2\alpha_m)\}_{i=1,2,\ldots,M_m}$ is a covering of $\mathcal{C}(\mathbf{z}; \gamma - \alpha_m)$. $\square$

5. Proof of the upper bound

The proof of Theorem 2 follows the proof of [2, Theorem 3.4] and uses two technical lemmas from [2, Lemmas 3.7–3.9], as well as a lemma that is analogous to [2, Lemma 3.2]. We first show the initial elementary steps of the proof of Theorem 2, and then introduce the necessary lemmas for the rest of the proof of Theorem 2.

Proof of Theorem 2 – Part I. Since $s > r/2$, the Sobolev space $H^s(\mathbb{S}^r)$ is a reproducing kernel Hilbert space (see Section 2.2) with reproducing kernel K_s given by (2.9). Thus for any bounded linear functional $\mathcal{L}$ on $H^s(\mathbb{S}^r)$, we have

$$\big(f, \mathcal{L}_2 K_s(\cdot, \cdot)\big)_s = \mathcal{L}f, \quad f \in H^s(\mathbb{S}^r), \tag{5.1}$$

where the index 2 in $\mathcal{L}_2$ indicates that $\mathcal{L}$ is applied to the second variable of $K_s(\cdot, \cdot)$. Since point evaluation and integration over $\mathcal{C}(\mathbf{z}; \gamma)$ are bounded linear functionals on $H^s(\mathbb{S}^r)$, using (2.8) and (5.1), the integration error of $Q_{m(n)}$ for an arbitrary function $f \in H^s(\mathbb{S}^r)$ can be written as

$$\left|Q_{m(n)}[f] - I_{\mathcal{C}(\mathbf{z};\gamma)}[f]\right| = \left|\left(f, \sum_{j=1}^{m(n)} w_j K_s(\cdot, \mathbf{x}_j) - \int_{\mathcal{C}(\mathbf{z};\gamma)} K_s(\cdot, \mathbf{x})\, \mathrm{d}\omega_r(\mathbf{x})\right)_s\right|.$$

From the Cauchy–Schwarz inequality, we find

$$\left|Q_{m(n)}[f] - I_{\mathcal{C}(\mathbf{z};\gamma)}[f]\right| \leq \|f\|_s \left\|\sum_{j=1}^{m(n)} w_j K_s(\cdot, \mathbf{x}_j) - \int_{\mathcal{C}(\mathbf{z};\gamma)} K_s(\cdot, \mathbf{x})\, \mathrm{d}\omega_r(\mathbf{x})\right\|_s, \tag{5.2}$$

and by choosing $f = h/\|h\|_s$ with $h = \sum_{j=1}^{m(n)} w_j K_s(\cdot, \mathbf{x}_j) - \int_{\mathcal{C}(\mathbf{z};\gamma)} K_s(\cdot, \mathbf{x})\, \mathrm{d}\omega_r(\mathbf{x})$ we obtain equality in (5.2). Thus the worst-case error of $Q_{m(n)}$, given by (1.4) with $H = H^s(\mathbb{S}^r)$, can be written as

$$E\big(Q_{m(n)}; H^s(\mathbb{S}^r)\big) = \left\|\sum_{j=1}^{m(n)} w_j K_s(\cdot, \mathbf{x}_j) - \int_{\mathcal{C}(\mathbf{z};\gamma)} K_s(\cdot, \mathbf{x})\, \mathrm{d}\omega_r(\mathbf{x})\right\|_s.$$

Noting that $\|g\|_s^2 = (g, g)_s$ for all $g \in H^s(\mathbb{S}^r)$ and using (2.8) and (5.1), we find

$$\begin{aligned}\big[E\big(Q_{m(n)}; H^s(\mathbb{S}^r)\big)\big]^2 &= \sum_{j=1}^{m(n)}\sum_{i=1}^{m(n)} w_j w_i K_s(\mathbf{x}_i, \mathbf{x}_j) - 2\sum_{j=1}^{m(n)} w_j \int_{\mathcal{C}(\mathbf{z};\gamma)} K_s(\mathbf{x}, \mathbf{x}_j)\, \mathrm{d}\omega_r(\mathbf{x}) \\ &\quad + \int_{\mathcal{C}(\mathbf{z};\gamma)}\int_{\mathcal{C}(\mathbf{z};\gamma)} K_s(\mathbf{x}, \mathbf{y})\, \mathrm{d}\omega_r(\mathbf{x})\, \mathrm{d}\omega_r(\mathbf{y}).\end{aligned} \tag{5.3}$$

The expansion (2.9) of the reproducing kernel K_s can be split it into a finite sum containing the spherical harmonic contributions of degree $\leq n$ and into a remainder term:

$$K_s(\mathbf{x},\mathbf{y}) = \kappa_s(\mathbf{x},\mathbf{y}) + K_s^{(n+1)}(\mathbf{x},\mathbf{y}), \quad \mathbf{x},\mathbf{y} \in \mathbb{S}^r, \tag{5.4}$$

where

$$\kappa_s(\mathbf{x},\mathbf{y}) := \sum_{\ell=0}^{n} \left(\ell + \frac{r-1}{2}\right)^{-2s} \frac{Z(r,\ell)}{|\mathbb{S}^r|} P_\ell(r+1; \mathbf{x}\cdot\mathbf{y}),$$

$$K_s^{(n+1)}(\mathbf{x},\mathbf{y}) := \sum_{\ell=n+1}^{\infty} \left(\ell + \frac{r-1}{2}\right)^{-2s} \frac{Z(r,\ell)}{|\mathbb{S}^r|} P_\ell(r+1; \mathbf{x}\cdot\mathbf{y}).$$

Since the function $\kappa_s(\mathbf{x},\mathbf{y})$ is in each variable a spherical polynomial of degree n, it is integrated exactly by the rule $Q_{m(n)}$. Hence,

$$\sum_{j=1}^{m(n)} w_j \int_{\mathcal{C}(\mathbf{z};\gamma)} \kappa_s(\mathbf{x},\mathbf{x}_j)\, \mathrm{d}\omega_r(\mathbf{x}) = \int_{\mathcal{C}(\mathbf{z};\gamma)} \int_{\mathcal{C}(\mathbf{z};\gamma)} \kappa_s(\mathbf{x},\mathbf{y})\, \mathrm{d}\omega_r(\mathbf{y})\, \mathrm{d}\omega_r(\mathbf{x}), \tag{5.5}$$

$$\sum_{j=1}^{m(n)} w_j \int_{\mathcal{C}(\mathbf{z};\gamma)} \kappa_s(\mathbf{x},\mathbf{x}_j)\, \mathrm{d}\omega_r(\mathbf{x}) = \sum_{j=1}^{m(n)} w_j \sum_{i=1}^{m(n)} w_i \kappa_s(\mathbf{x}_i,\mathbf{x}_j). \tag{5.6}$$

Substituting (5.4) into (5.3) and making use of (5.5) and (5.6), all contributions involving κ_s cancel, and the squared worst-case error is given by

$$\begin{aligned}\left[E\left(Q_{m(n)}; H^s(\mathbb{S}^r)\right)\right]^2 &= \sum_{j=1}^{m(n)} \sum_{i=1}^{m(n)} w_j w_i K_s^{(n+1)}(\mathbf{x}_i,\mathbf{x}_j) - 2 \sum_{j=1}^{m(n)} w_j \int_{\mathcal{C}(\mathbf{z};\gamma)} K_s^{(n+1)}(\mathbf{x},\mathbf{x}_j)\, \mathrm{d}\omega_r(\mathbf{x}) \\ &\quad + \int_{\mathcal{C}(\mathbf{z};\gamma)} \int_{\mathcal{C}(\mathbf{z};\gamma)} K_s^{(n+1)}(\mathbf{x},\mathbf{y})\, \mathrm{d}\omega_r(\mathbf{x})\, \mathrm{d}\omega_r(\mathbf{y}).\end{aligned} \tag{5.7}$$

The rest of the proof will be given once the required lemmas have been introduced. □

The following two lemmas from [2, Lemmas 3.7, 3.8, and 3.9] and the rest of the proof of Theorem 2 use the *Pochhammer symbol*: for $z \in \mathbb{R} \setminus \{-1,-2,\ldots\}$,

$$(z)_0 := 1 \quad \text{and} \quad (z)_\ell := z\cdot(z+1)\cdot\ldots\cdot(z+\ell-1) = \frac{\Gamma(z+\ell)}{\Gamma(z)}, \quad \ell \in \mathbb{N}.$$

Lemma 6. *Let $r \geq 2$, $s > r/2$, and let $L \in \mathbb{N}$ be fixed. For $-1 \leq t \leq 1$, we have pointwise*

$$\begin{aligned}&\sum_{\ell=n+1}^{\infty} \left(\ell + \frac{r-1}{2}\right)^{-2s} \frac{Z(r,\ell)}{|\mathbb{S}^r|} P_\ell(r+1;t) \\ &= -\frac{1}{|\mathbb{S}^r|} \sum_{k=0}^{L-1} \lambda_{n+1}^{(k)} \frac{(r+k)_n}{(r/2)_n} P_n^{((r-2)/2+k+1,(r-2)/2)}(t) \\ &\quad + \frac{1}{|\mathbb{S}^r|} \sum_{\ell=n+1}^{\infty} \lambda_\ell^{(L)} \frac{(2\ell+r-1+L)}{(r-1+L)} \frac{(r-1+L)_\ell}{(r/2)_\ell} P_\ell^{((r-2)/2+L,(r-2)/2)}(t),\end{aligned} \tag{5.8}$$

where the coefficients $\lambda_\ell^{(k)}$, $\ell \in \mathbb{N}_0$, $k = 0,1,\ldots,L$, are defined recursively by

$$\lambda_\ell^{(0)} := \left(\ell + \frac{r-1}{2}\right)^{-2s} \quad \textit{and} \quad \lambda_\ell^{(k+1)} := \frac{r+k}{2\ell+r+k}\left(\lambda_\ell^{(k)} - \lambda_{\ell+1}^{(k)}\right), \quad k \in \mathbb{N}_0. \tag{5.9}$$

The coefficients $\lambda_\ell^{(k)}$, $\ell \in \mathbb{N}_0$, $k = 0, 1, \ldots, L$, *satisfy*

$$c_1 \ell^{-2k-2s} \leq \lambda_\ell^{(k)} \leq c_2 \ell^{-2k-2s}, \tag{5.10}$$

with positive constants c_1 *and* c_2 *that depend only on* r, s, *and* L.

In the rest of the proof of Theorem 2, (5.8) is used to split $K_s^{(n+1)}$ into a polynomial part of degree $\leq n$, given by the first term on the right-hand side of (5.8), which is integrated exactly by the numerical integration rule $Q_{m(n)}$, and into an infinite remainder series, given by the second term on the right-hand side of (5.8). With the help of the next lemma, it is possible to estimate the contribution of this infinite remainder series to the squared worst-case error.

Lemma 7. *Let* $r \geq 2$, $s > r/2$, *let* $L \in \mathbb{N}$ *be fixed, and let* $\lambda_\ell^{(k)}$ *be defined recursively by* (5.9). *There exists a positive constant* c_3 *such that for any* $n \in \mathbb{N}$ *and for all* $-1 \leq t \leq 1$,

$$\left| \frac{1}{|\mathbb{S}^r|} \sum_{\ell=n+1}^{\infty} \lambda_\ell^{(L)} \frac{(2\ell + r - 1 + L)}{(r - 1 + L)} \frac{(r - 1 + L)_\ell}{(r/2)_\ell} P_\ell^{((r-2)/2+L,(r-2)/2)}(t) \right| \leq c_3 n^{r-2s}. \tag{5.11}$$

There exists a positive constant c_4 *such that for any* $n \in \mathbb{N}$ *and for all* θ *satisfying* $0 < \theta < \pi$,

$$\left| \frac{1}{|\mathbb{S}^r|} \sum_{\ell=n+1}^{\infty} \lambda_\ell^{(L)} \frac{(2\ell + r - 1 + L)}{(r - 1 + L)} \frac{(r - 1 + L)_\ell}{(r/2)_\ell} P_\ell^{((r-2)/2+L,(r-2)/2)}(\cos\theta) \right|$$
$$\leq c_4 n^{(r+1)/2-L-2s} (\sin\theta)^{-(r-1)/2-L}. \tag{5.12}$$

The positive constants c_3 *and* c_4 *in* (5.11) *and* (5.12) *depend only on* r, s, *and* L.

Lemma 7 is proved analogously to [2, Lemma 3.9], using [22, (7.32.6) and (4.1.3)]. (Note that the second estimate in [2, Lemma 3.9] is slightly different from (5.12).)

Finally we need the following technical lemma which will be proved at the end of this section.

Lemma 8. *Let* $\gamma \in (0, \pi]$. *Consider a rule* $Q_m[f] := \sum_{j=1}^m w_j f(\mathbf{x}_j)$ *for numerical integration over* $\mathcal{C}(\mathbf{z}; \gamma) \subset \mathbb{S}^r$, *with real weights* w_j *and nodes* $\mathbf{x}_j \in \mathcal{C}(\mathbf{z}; \gamma)$. *If there exists a positive constant* C *and a radius* $\beta \leq \min\{\gamma, \pi/2\}$ *such that*

$$\sum_{\substack{j=1, \\ \mathbf{x}_j \in \mathcal{C}(\mathbf{y};\beta)}}^{m} |w_j| \leq C\beta^r \quad \textit{for all } \mathbf{y} \in \mathbb{S}^r, \tag{5.13}$$

then for all radii θ *with* $\theta \in [\beta, \pi/2]$

$$\sum_{\substack{j=1, \\ \mathbf{x}_j \in \mathcal{C}(\mathbf{y};\theta)}}^{m} |w_j| \leq C 2^{1-r} 3^r \pi^{2r-1} \big(\sin(\min\{\theta, \gamma\})\big)^r \quad \textit{for all } \mathbf{y} \in \mathbb{S}^r, \tag{5.14}$$

where the constant C *in* (5.14) *is the same constant* C *as in* (5.13).

Proof of Theorem 2 – Part II. From the split (5.8) given in Lemma 6 we find

$$K_s^{(n+1)}(\mathbf{x}, \mathbf{y}) = -\frac{1}{|\mathbb{S}^r|} \sum_{k=0}^{L-1} \lambda_{n+1}^{(k)} \frac{(r+k)_n}{(r/2)_n} P_n^{((r-2)/2+k+1,(r-2)/2)}(\mathbf{x} \cdot \mathbf{y})$$
$$+ \frac{1}{|\mathbb{S}^r|} \sum_{\ell=n+1}^{\infty} \lambda_\ell^{(L)} \frac{(2\ell + r - 1 + L)}{(r - 1 + L)} \frac{(r - 1 + L)_\ell}{(r/2)_\ell} P_\ell^{((r-2)/2+L,(r-2)/2)}(\mathbf{x} \cdot \mathbf{y}), \tag{5.15}$$

where the integer L is chosen fixed such that $L > (r+1)/2$. The first finite sum in (5.15) is a spherical polynomial of degree $\leq n$ with respect to each variable $\mathbf{x}$ and $\mathbf{y}$, and, with the same argumentation that we used for κ_s, all contributions in (5.7) from this finite sum cancel. Thus we obtain from (5.7) that the squared worst-case error is given by

$$\left[E\left(Q_{m(n)}; H^s(\mathbb{S}^r)\right)\right]^2 = \sum_{j=1}^{m(n)} \sum_{i=1}^{m(n)} w_j w_i \widetilde{K}_s^{(n+1)}(\mathbf{x}_i, \mathbf{x}_j) - 2 \sum_{j=1}^{m(n)} w_j \int_{\mathcal{C}(\mathbf{z};\gamma)} \widetilde{K}_s^{(n+1)}(\mathbf{x}, \mathbf{x}_j)\, \mathrm{d}\omega_r(\mathbf{x}) + \int_{\mathcal{C}(\mathbf{z};\gamma)} \int_{\mathcal{C}(\mathbf{z};\gamma)} \widetilde{K}_s^{(n+1)}(\mathbf{x}, \mathbf{y})\, \mathrm{d}\omega_r(\mathbf{x})\, \mathrm{d}\omega_r(\mathbf{y}), \tag{5.16}$$

with $\widetilde{K}_s^{(n+1)}$ defined by the infinite sum

$$\widetilde{K}_s^{(n+1)}(\mathbf{x}, \mathbf{y}) := \frac{1}{|\mathbb{S}^r|} \sum_{\ell=n+1}^{\infty} \lambda_\ell^{(L)} \frac{(2\ell + r - 1 + L)}{(r - 1 + L)} \frac{(r - 1 + L)_\ell}{(r/2)_\ell} P_\ell^{((r-2)/2+L,(r-2)/2)}(\mathbf{x} \cdot \mathbf{y}).$$

From Lemma 7 we obtain the following two estimates for $\widetilde{K}_s^{(n+1)}$: from (5.11)

$$\sup_{\mathbf{x},\mathbf{y}\in\mathbb{S}^r} |\widetilde{K}_s^{(n+1)}(\mathbf{x}, \mathbf{y})| \le c_3 n^{r-2s}, \tag{5.17}$$

and with the notation $\mathbf{x} \cdot \mathbf{y} = \cos\theta$, with $\theta \in [0, \pi]$, we obtain from (5.12)

$$|\widetilde{K}_s^{(n+1)}(\mathbf{x}, \mathbf{y})| \le c_4 n^{(r+1)/2-L-2s} (\sin\theta)^{-(r-1)/2-L}, \quad \theta \in (0, \pi). \tag{5.18}$$

We obtain an upper bound of $[E(Q_{m(n)}; H^s(\mathbb{S}^r))]^2$ by taking in (5.16) absolute values.

$$\left[E\left(Q_{m(n)}; H^s(\mathbb{S}^r)\right)\right]^2 \le \sum_{j=1}^{m(n)} \sum_{i=1}^{m(n)} |w_j||w_i||\widetilde{K}_s^{(n+1)}(\mathbf{x}_i, \mathbf{x}_j)| + 2 \sum_{j=1}^{m(n)} |w_j| \int_{\mathcal{C}(\mathbf{z};\gamma)} |\widetilde{K}_s^{(n+1)}(\mathbf{x}, \mathbf{x}_j)|\, \mathrm{d}\omega_r(\mathbf{x}) + \int_{\mathcal{C}(\mathbf{z};\gamma)} \int_{\mathcal{C}(\mathbf{z};\gamma)} |\widetilde{K}_s^{(n+1)}(\mathbf{x}, \mathbf{y})|\, \mathrm{d}\omega_r(\mathbf{x})\, \mathrm{d}\omega_r(\mathbf{y}). \tag{5.19}$$

Now we use (5.17) and (5.18) to estimate the three terms in (5.19). For any $\mathbf{y} \in \mathcal{C}(\mathbf{z}; \gamma)$, we have

$$\int_{\mathcal{C}(\mathbf{z};\gamma)} |\widetilde{K}_s^{(n+1)}(\mathbf{x}, \mathbf{y})|\, \mathrm{d}\omega_r(\mathbf{x}) \le \int_{\mathbb{S}^r} |\widetilde{K}_s^{(n+1)}(\mathbf{x}, \mathbf{y})|\, \mathrm{d}\omega_r(\mathbf{x}) \le S^- + S^+ + T^- + T^+, \tag{5.20}$$

where

$$S^\pm := \int_{\mathcal{C}(\pm\mathbf{y};\gamma/(\pi n))} |\widetilde{K}_s^{(n+1)}(\mathbf{x}, \mathbf{y})|\, \mathrm{d}\omega_r(\mathbf{x}),$$

$$T^\pm := \int_{\mathcal{C}(\pm\mathbf{y};\pi/2)\setminus\mathcal{C}(\pm\mathbf{y};\gamma/(\pi n))} |\widetilde{K}_s^{(n+1)}(\mathbf{x}, \mathbf{y})|\, \mathrm{d}\omega_r(\mathbf{x}).$$

In words, the whole sphere is written as a union of a north polar cap $\mathcal{C}(\mathbf{y}; \gamma/(\pi n))$ and a south polar cap $\mathcal{C}(-\mathbf{y}; \gamma/(\pi n))$ with respect to $\mathbf{y}$ as the north pole and the remainder of the corresponding northern and southern hemispheres. To estimate S^+ and S^-, we use (5.17) and (2.2)

$$S^\pm \le c_3 n^{r-2s} \int_{\mathcal{C}(\pm\mathbf{y};\gamma/(\pi n))} \mathrm{d}\omega_r(\mathbf{x}) \le c_3 n^{r-2s} \frac{|\mathbb{S}^{r-1}|}{r} \left(\frac{\gamma}{\pi n}\right)^r \le c_3 \frac{|\mathbb{S}^{r-1}|\gamma^r}{\pi^r r} n^{-2s} \le c_3 \frac{2}{\pi} |\mathcal{C}(\mathbf{z}; \gamma)| n^{-2s}. \tag{5.21}$$

As $K_s^{(n+1)}(\mathbf{x}, \mathbf{y})$ depends only on $\mathbf{x} \cdot \mathbf{y}$, (2.1) can be used to parameterize the integral $T^\pm$. From the subsequent substitution $t = \mathbf{x} \cdot \mathbf{y} = \cos\theta$, $\theta \in [0, \pi]$, and the estimate (5.18),

$$T^\pm \le c_4 |\mathbb{S}^{r-1}| n^{(r+1)/2-L-2s} \int_{\gamma/(\pi n)}^{\pi/2} \left(\sin\theta\right)^{(r-1)/2-L} \mathrm{d}\theta. \tag{5.22}$$

Since by assumption $L > (r+1)/2$ and since $\sin\theta \geq 2\theta/\pi$ for all $\theta \in [0, \pi/2]$,

$$\begin{aligned}\int_{\gamma/(\pi n)}^{\pi/2} \big(\sin\theta\big)^{(r-1)/2-L}\, \mathrm{d}\theta &\leq \left(\frac{2}{\pi}\right)^{(r-1)/2-L} \int_{\gamma/(\pi n)}^{\pi/2} \theta^{(r-1)/2-L}\, \mathrm{d}\theta \\ &= \left(\frac{2}{\pi}\right)^{(r-1)/2-L} \frac{\theta^{(r+1)/2-L}}{(r+1)/2-L}\Bigg|_{\gamma/(\pi n)}^{\pi/2} \\ &\leq \frac{(2/\pi)^{(r-1)/2-L}}{L-(r+1)/2}\left(\frac{\gamma}{\pi n}\right)^{(r+1)/2-L} \\ &= \frac{2^{(r+1)/2-L}\pi^{2L-r}\gamma^{(r+1)/2-L}}{2L-(r+1)} n^{L-(r+1)/2}. \end{aligned} \tag{5.23}$$

Combining (5.22) and (5.23) and using the upper bound in (2.2) yields

$$\begin{aligned} T^{\pm} &\leq c_4 \frac{2^{(r+1)/2-L}\pi^{2L-r}|\mathbb{S}^{r-1}|\gamma^{(r+1)/2-L}}{2L-(r+1)} n^{-2s} \\ &\leq c_4 \frac{2^{(r+1)/2-L}\pi^{2L-r}|\mathbb{S}^{r-1}|^{1/2+L/r-1/(2r)}}{(2L-(r+1))r^{(L-(r+1)/2)/r}} |\mathcal{C}(\mathbf{z};\gamma)|^{((r+1)/2-L)/r} n^{-2s}. \end{aligned} \tag{5.24}$$

From (5.20), (5.21) and (5.24), for all $\mathbf{y} \in \mathbb{S}^r$,

$$\begin{aligned} &\int_{\mathcal{C}(\mathbf{z};\gamma)} |\widetilde{K}_s^{(n+1)}(\mathbf{x},\mathbf{y})|\, \mathrm{d}\omega_r(\mathbf{x}) \\ &\leq \left(c_3 \frac{4}{\pi}|\mathcal{C}(\mathbf{z};\gamma)| + c_4 \frac{2^{(r+3)/2-L}\pi^{2L-r}|\mathbb{S}^{r-1}|^{1/2+L/r-1/(2r)}}{(2L-(r+1))r^{(L-(r+1)/2)/r}}|\mathcal{C}(\mathbf{z};\gamma)|^{((r+1)/2-L)/r}\right) n^{-2s}. \end{aligned} \tag{5.25}$$

The estimate (5.25) implies immediately that the last term in (5.19) is of the order n^{-2s}, as

$$\begin{aligned} &\int_{\mathcal{C}(\mathbf{z};\gamma)} \int_{\mathcal{C}(\mathbf{z};\gamma)} |\widetilde{K}_s^{(n+1)}(\mathbf{x},\mathbf{y})|\, \mathrm{d}\omega_r(\mathbf{x})\, \mathrm{d}\omega_r(\mathbf{y}) \\ &\leq \left(c_3 \frac{4}{\pi}|\mathcal{C}(\mathbf{z};\gamma)|^2 + c_4 \frac{2^{(r+3)/2-L}\pi^{2L-r}|\mathbb{S}^{r-1}|^{1/2+L/r-1/(2r)}}{(2L-(r+1))r^{(L-(r+1)/2)/r}}|\mathcal{C}(\mathbf{z};\gamma)|^{1+((r+1)/2-L)/r}\right) n^{-2s}. \end{aligned} \tag{5.26}$$

To estimate the other two terms we exploit that the regularity condition (3.2) on the sequence $\{Q_{m(n)}\}_{n\in\mathbb{N}}$ and Lemma 8 imply that the weights w_j and nodes $\mathbf{x}_j$ of the rule $Q_{m(n)}$ satisfy

$$\sum_{\substack{j=1,\\ \mathbf{x}_j\in\mathcal{C}(\mathbf{y};\theta)}}^{m(n)} |w_j| \leq C 2^{1-r}3^r\pi^{2r-1}\big(\sin(\min\{\theta,\gamma\})\big)^r \quad \text{for all } \mathbf{y}\in\mathbb{S}^r \text{ and all } \theta \in \left[\frac{\gamma}{\pi n}, \frac{\pi}{2}\right], \tag{5.27}$$

where the constant C is the constant from (3.2). In particular, from applying (5.27) for $\mathcal{C}(\mathbf{z};\pi/2)$ and $\mathcal{C}(-\mathbf{z};\pi/2))$ and using $\sin\phi \leq \phi$ for all $\phi \in [0,\pi]$ and the lower bound in (2.2)

$$\begin{aligned} \sum_{j=1}^{m(n)} |w_j| &\leq C 2^{2-r}3^r\pi^{2r-1}\big(\sin(\min\{\pi/2,\gamma\})\big)^r \leq C 2^{2-r}3^r\pi^{2r-1}\big(\min\{\pi/2,\gamma\}\big)^r \\ &\leq C 2^{2-r}3^r\pi^{2r-1}\gamma^r \leq C \frac{2^{3-r}3^r\pi^{3r-2}r}{|\mathbb{S}^{r-1}|}|\mathcal{C}(\mathbf{z};\gamma)|. \end{aligned} \tag{5.28}$$

The estimates (5.25) and (5.28) show that the second term in (5.19) is of the order n^{-2s}, as

$$\sum_{j=1}^{m(n)} |w_j| \int_{\mathcal{C}(\mathbf{z};\gamma)} |\widetilde{K}_s^{(n+1)}(\mathbf{x}, \mathbf{x}_j)|\, \mathrm{d}\omega_r(\mathbf{x}) \le C \frac{2^{3-r} 3^r \pi^{3r-2} r}{|\mathbb{S}^{r-1}|} \times \left(c_3 \frac{4}{\pi} |\mathcal{C}(\mathbf{z};\gamma)|^2 + c_4 \frac{2^{(r+3)/2-L} \pi^{2L-r} |\mathbb{S}^{r-1}|^{1/2+L/r-1/(2r)}}{(2L-(r+1)) r^{(L-(r+1)/2)/r}} |\mathcal{C}(\mathbf{z};\gamma)|^{1+((r+1)/2-L)/r} \right) n^{-2s}. \tag{5.29}$$

To estimate the first term in (5.19), we bound it by the following four components:

$$\sum_{j=1}^{m(n)} \sum_{i=1}^{m(n)} |w_j||w_i||\widetilde{K}_s^{(n+1)}(\mathbf{x}_i, \mathbf{x}_j)| \le D^+ + D^- + R^+ + R^-, \tag{5.30}$$

where

$$D^{\pm} := \sum_{j=1}^{m(n)} |w_j| \sum_{\substack{i=1,\\ \mathbf{x}_i \in \mathcal{C}(\pm \mathbf{x}_j;\gamma/(\pi n))}}^{m(n)} |w_i||\widetilde{K}_s^{(n+1)}(\mathbf{x}_i, \mathbf{x}_j)|,$$

$$R^{\pm} := \sum_{j=1}^{m(n)} |w_j| \sum_{\substack{i=1,\\ \mathbf{x}_i \in \mathcal{C}(\pm \mathbf{x}_j;\pi/2),\\ \mathbf{x}_i \notin \mathcal{C}(\pm \mathbf{x}_j;\gamma/(\pi n))}}^{m(n)} |w_i|\, |\widetilde{K}_s^{(n+1)}(\mathbf{x}_i, \mathbf{x}_j)|.$$

From (5.17), the regularity condition (3.2) and (5.28), and the lower bound in (2.2)

$$\begin{aligned} D^{\pm} &\le c_3 n^{r-2s} \sum_{j=1}^{m(n)} |w_j| \sum_{\substack{i=1,\\ \mathbf{x}_i \in \mathcal{C}(\pm \mathbf{x}_j;\gamma/(\pi n))}}^{m(n)} |w_i| \\ &\le c_3 n^{r-2s} \sum_{j=1}^{m(n)} |w_j| C \left(\frac{\gamma}{\pi n}\right)^r \le c_3 C \pi^{-r} \gamma^r n^{-2s} \sum_{j=1}^{m(n)} |w_j| \\ &\le c_3 C^2 \frac{2^{3-r} 3^r \pi^{2r-2} r \gamma^r}{|\mathbb{S}^{r-1}|} |\mathcal{C}(\mathbf{z};\gamma)| n^{-2s} \le c_3 C^2 \frac{2^{4-r} 3^r \pi^{3r-3} r^2}{|\mathbb{S}^{r-1}|^2} |\mathcal{C}(\mathbf{z};\gamma)|^2 n^{-2s}. \end{aligned} \tag{5.31}$$

From (5.18), we have with $\theta_{i,j} := \arccos(\mathbf{x}_i \cdot \mathbf{x}_j)$, $\theta_{i,j} \in [0, \pi]$,

$$R^{\pm} \le c_4 n^{(r+1)/2-L-2s} \sum_{j=1}^{m(n)} |w_j| \sum_{\substack{i=1,\\ \mathbf{x}_i \in \mathcal{C}(\pm \mathbf{x}_j;\pi/2),\\ \mathbf{x}_i \notin \mathcal{C}(\pm \mathbf{x}_j;\gamma/(\pi n))}}^{m(n)} |w_i| (\sin \theta_{i,j})^{-(r-1)/2-L}. \tag{5.32}$$

Following exactly the steps taken in [2, pages 57–59] (using ideas from [19]), we find

$$\begin{aligned} \sum_{\substack{i=1,\\ \mathbf{x}_i \in \mathcal{C}(\pm \mathbf{x}_j;\pi/2),\\ \mathbf{x}_i \notin \mathcal{C}(\pm \mathbf{x}_j;\gamma/(\pi n))}}^{m(n)} |w_i| (\sin \theta_{i,j})^{-(r-1)/2-L} &\le C 2^{(5-r)/2-L} 3^r \pi^{2L+r-2} \frac{(r-1)/2+L}{L-(r+1)/2} \gamma^{(r+1)/2-L} n^{L-(r+1)/2} \\ &\le C \frac{2^{(5-r)/2-L} 3^r \pi^{2L+r-2} \left(\frac{r-1}{2}+L\right)}{|\mathbb{S}^{r-1}|^{((r+1)/2-L)/r} r^{(L-(r+1)/2)/r} \left(L-\frac{r+1}{2}\right)} |\mathcal{C}(\mathbf{z};\gamma)|^{((r+1)/2-L)/r} n^{L-(r+1)/2}, \end{aligned} \tag{5.33}$$

where the upper bound in (2.2) was used in the last step. Applying (5.33) to the inner sum in (5.32) and using (5.28) yields

$$\begin{aligned} R^{\pm} &\leq c_4 C \frac{2^{(5-r)/2-L} 3^r \pi^{2L+r-2} \left(\frac{r-1}{2}+L\right)}{|\mathbb{S}^{r-1}|^{((r+1)/2-L)/r} r^{(L-(r+1)/2)/r} \left(L-\frac{r+1}{2}\right)} |\mathcal{C}(\mathbf{z};\gamma)|^{((r+1)/2-L)/r} n^{-2s} \sum_{j=1}^{m(n)} |w_j| \\ &\leq c_4 C^2 \frac{2^{(11-3r)/2-L} 3^{2r} \pi^{2L+4r-4} \left(\frac{r-1}{2}+L\right)}{|\mathbb{S}^{r-1}|^{1+((r+1)/2-L)/r} r^{-1+(L-(r+1)/2)/r} \left(L-\frac{r+1}{2}\right)} |\mathcal{C}(\mathbf{z};\gamma)|^{1+((r+1)/2-L)/r} n^{-2s}. \end{aligned} \tag{5.34}$$

Applying (5.31) and (5.34) in (5.30) yields

$$\begin{aligned} \sum_{j=1}^{m(n)} \sum_{i=1}^{m(n)} |w_i||w_j||\widetilde{K}_s^{(n+1)}(\mathbf{x}_i,\mathbf{x}_j)| &\leq c_3 C^2 \frac{2^{5-r} 3^r \pi^{3r-3} r^2}{|\mathbb{S}^{r-1}|^2} |\mathcal{C}(\mathbf{z};\gamma)|^2 n^{-2s} \\ &+ c_4 C^2 \frac{2^{(13-3r)/2-L} 3^{2r} \pi^{2L+4r-4} \left(\frac{r-1}{2}+L\right)}{|\mathbb{S}^{r-1}|^{1+((r+1)/2-L)/r} r^{-1+(L-(r+1)/2)/r} \left(L-\frac{r+1}{2}\right)} |\mathcal{C}(\mathbf{z};\gamma)|^{1+((r+1)/2-L)/r} n^{-2s}. \end{aligned} \tag{5.35}$$

From (5.19), (5.26), (5.29) and (5.35), we conclude that

$$\left[E(Q_{m(n)}; H^s(\mathbb{S}^r))\right]^2 \leq \tilde{c}_{r,s} |\mathcal{C}(\mathbf{z};\gamma)|^{1+((r+1)/2-L)/r} n^{-2s}, \tag{5.36}$$

with a positive constant $\tilde{c}_{r,s}$ that depends only on r and s and the constant C from the regularity property (3.2). By choosing the fixed integer constant L with $L > (r+1)/2$ in (5.36) as $L = \lfloor (r+1)/2 \rfloor + 1$, we obtain (3.3) in Theorem 2. □

Proof of Lemma 8. First we note that, in the estimate (5.14), we may replace under the summation sign $\mathbf{x}_j \in \mathcal{C}(\mathbf{y};\theta)$ by $\mathbf{x}_j \in \mathcal{C}(\mathbf{y};\theta) \cap \mathcal{C}(\mathbf{z};\gamma)$, since all nodes $\mathbf{x}_j$ lie in $\mathcal{C}(\mathbf{z};\gamma)$.

Let $\mathbf{y}$ be an arbitrary point on $\mathbb{S}^r$, and let $\theta \in [\beta, \pi/2]$. Let $\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N$ be a *maximal* set of points in $\mathcal{C}(\mathbf{y};\theta) \cap \mathcal{C}(\mathbf{z};\gamma)$ with $\operatorname{dist}(\mathbf{z}_i,\mathbf{z}_j) \geq \beta$ for $i \neq j$. Then the spherical caps $\mathcal{C}(\mathbf{z}_i;\beta/2)$, $i = 1, 2, \ldots, N$, touch each other at most at the boundary, and they are all contained in $\mathcal{C}(\mathbf{y};\theta+\beta/2) \cap \mathcal{C}(\mathbf{z};\min\{\gamma+\beta/2,\pi\})$. Thus

$$\sum_{i=1}^{N} \left|\mathcal{C}\big(\mathbf{z}_i;\beta/2\big)\right| = N\left|\mathcal{C}\big(\mathbf{z}_1;\beta/2\big)\right| \leq \left|\mathcal{C}\big(\mathbf{y};\theta+\beta/2\big) \cap \mathcal{C}\big(\mathbf{z};\min\{\gamma+\beta/2,\pi\}\big)\right|.$$

It is easily seen that

$$\left|\mathcal{C}\big(\mathbf{y};\theta+\beta/2\big) \cap \mathcal{C}\big(\mathbf{z};\min\{\gamma+\beta/2,\pi\}\big)\right| \leq \left|\mathcal{C}\big(\mathbf{z};\min\{\theta,\gamma\}+\beta/2\big)\right|.$$

Hence, the number of points N has the upper bound

$$N \leq \frac{\left|\mathcal{C}\big(\mathbf{z};\min\{\theta,\gamma\}+\beta/2\big)\right|}{\left|\mathcal{C}\big(\mathbf{z}_1;\beta/2\big)\right|}. \tag{5.37}$$

Because the points $\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N \in \mathcal{C}(\mathbf{y};\theta) \cap \mathcal{C}(\mathbf{z};\gamma)$ form a *maximal* set with the property $\operatorname{dist}(\mathbf{z}_i,\mathbf{z}_j) \geq \beta$ for $i \neq j$, the spherical caps $\mathcal{C}(\mathbf{z}_i;\beta)$, $i = 1, 2, \ldots, N$, form a covering of $\mathcal{C}(\mathbf{y};\theta) \cap \mathcal{C}(\mathbf{z};\gamma)$. (Indeed, assume that $\{\mathcal{C}(\mathbf{z}_i;\beta)\}_{i=1,2,\ldots,N}$, is not a covering of $\mathcal{C}(\mathbf{y};\theta) \cap \mathcal{C}(\mathbf{z};\gamma)$. Then there exists a point $\mathbf{u} \in \mathcal{C}(\mathbf{y};\theta) \cap \mathcal{C}(\mathbf{z};\gamma)$ that is not contained in any cap $\mathcal{C}(\mathbf{z}_i;\beta)$, $i = 1, 2, \ldots, N$, that is, $\operatorname{dist}(\mathbf{u},\mathbf{z}_i) > \beta$ for all $i = 1, 2, \ldots, N$. This is a contradiction to the fact that the set $\{\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N\} \subset \mathcal{C}(\mathbf{y};\theta) \cap \mathcal{C}(\mathbf{z};\gamma)$, with $\operatorname{dist}(\mathbf{z}_i,\mathbf{z}_j) \geq \beta$ for $i \neq j$, was maximal.) Since the spherical caps $\mathcal{C}(\mathbf{z}_i;\beta)$, $i = 1, 2, \ldots, N$, form a covering of $\mathcal{C}(\mathbf{y};\theta) \cap \mathcal{C}(\mathbf{z};\gamma)$, we have from the assumption (5.13)

$$\sum_{\substack{j=1,\\ \mathbf{x}_j \in \mathcal{C}(\mathbf{y};\theta)}}^{m} |w_j| = \sum_{\substack{j=1,\\ \mathbf{x}_j \in \mathcal{C}(\mathbf{y};\theta)\cap\mathcal{C}(\mathbf{z};\gamma)}}^{m} |w_j| \leq \sum_{i=1}^{N} \sum_{\substack{j=1,\\ \mathbf{x}_j \in \mathcal{C}(\mathbf{z}_i;\beta)}}^{m} |w_j| \leq \sum_{i=1}^{N} C\beta^r = CN\beta^r. \tag{5.38}$$

Estimating N in (5.38) by (5.37) and using (2.2) yields

$$\sum_{\substack{j=1,\\ \mathbf{x}_j\in\mathcal{C}(\mathbf{y};\theta)}}^{m} |w_j| \leq C\beta^r \frac{\left|\mathcal{C}\big(\mathbf{z};\min\{\theta,\gamma\}+\beta/2\big)\right|}{\left|\mathcal{C}\big(\mathbf{z}_1;\beta/2\big)\right|} \leq C2\pi^{r-1}\beta^r\frac{\big(\min\{\theta,\gamma\}+\beta/2\big)^r}{\big(\beta/2\big)^r}$$

$$\leq C2^{r+1}\pi^{r-1}\left(\frac{3}{2}\min\{\theta,\gamma\}\right)^r \leq C2^{1-r}3^r\pi^{2r-1}\big(\sin(\min\{\theta,\gamma\})\big)^r,$$

where we have used $\beta/2 \leq \theta/2$, $\beta/2 \leq \gamma/2$ and hence $\min\{\theta,\gamma\}+\beta/2 \leq (3/2)\min\{\theta,\gamma\}$, and $\min\{\theta,\gamma\} \leq \theta \leq \pi/2$ and $2\phi/\pi \leq \sin\phi$ for all $\phi \in [0,\pi/2]$. This proves (5.14). $\square$

6. Extension of the results to general subsets of the sphere

An inspection of the proofs shows that it is possible to extend the results to a *general closed and connected measurable subset $\Omega \subset \mathbb{S}^r$ that is the closure of an open set*. Let $|\Omega|$ denote the area of Ω. We choose spherical caps $\mathcal{C}(\mathbf{z}_1;\gamma_1)$ and $\mathcal{C}(\mathbf{z}_2;\gamma_2)$, with $\gamma_1,\gamma_2 \in (0,\pi]$, such that

$$\mathcal{C}(\mathbf{z}_1;\gamma_1) \subset \Omega \subset \mathcal{C}(\mathbf{z}_2;\gamma_2).$$

The spherical cap $\mathcal{C}(\mathbf{z}_1;\gamma_1)$ will be chosen as large as possible, so that it covers as much area of Ω as possible. Likewise the spherical cap $\mathcal{C}(\mathbf{z}_2;\gamma_2)$ will be chosen as small as possible. Bounds on the worst-case error in a (global) Sobolev space setting are now obtained by exploiting the given proofs for these two caps.

More precisely, let

$$I_\Omega[f] := \int_\Omega f(\mathbf{x})\,\mathrm{d}\omega_r(\mathbf{x}),$$

and consider a rule for numerical integration over Ω,

$$Q_m[f] := \sum_{j=1}^{m} w_j f(\mathbf{x}_j), \tag{6.1}$$

with real weights w_j, $j = 1,2,\ldots,m$, and nodes $\mathbf{x}_j$, $j = 1,2,\ldots,m$, located in the subset Ω. The aim is to estimate the worst-case error of the rule Q_m, given by (6.1), in $H^s(\mathbb{S}^r)$

$$E\big(Q_m;H^s(\mathbb{S}^r)\big) := \sup_{\substack{f\in H^s(\mathbb{S}^r),\\ \|f\|_s\leq 1}} \big|Q_m[f]-I_\Omega[f]\big|.$$

For obtaining a lower bound on the worst-case error, we consider a spherical cap $\mathcal{C}(\mathbf{z}_1;\gamma_1)$, with $\gamma_1 \in (0,\pi]$, contained in Ω (that is, $\mathcal{C}(\mathbf{z}_1;\gamma_1) \subset \Omega$) and construct the same 'bad function' f_m as in the proof of Theorem 1 for this cap $\mathcal{C}(\mathbf{z}_1;\gamma_1)$. Then

$$E\big(Q_m;H^s(\mathbb{S}^r)\big) \geq \frac{1}{\|f_m\|_s}\big|Q_m[f_m]-I_\Omega[f_m]\big| = \frac{1}{\|f_m\|_s}I_\Omega[f_m] = \frac{1}{\|f_m\|_s}I_{\mathcal{C}(\mathbf{z}_1;\gamma_1)}[f_m],$$

because the function f_m vanishes at the nodes of the rule Q_m and has non-negative values, and because the support of f_m is contained in $\mathcal{C}(\mathbf{z}_1;\gamma_1)$. Both factors on the right-hand side were estimated in the proof of Theorem 1, and we obtain the following theorem.

Theorem 9. *Let $r \geq 2$ and $s > r/2$. Let Ω be a non-empty closed and connected measurable subset of $\mathbb{S}^r$ that is the closure of an open set, and let $\mathcal{C}(\mathbf{z}_1;\gamma_1) \subset \Omega$ with $\gamma_1 \in (0,\pi]$. Then there exists a positive constant $c_{r,s}$ such that the worst-case error in $H^s(\mathbb{S}^r)$ of any rule Q_m for numerical integration over Ω, given by (6.1) with m nodes in Ω, satisfies*

$$E\big(Q_m;H^s(\mathbb{S}^r)\big) \geq c_{r,s}|\mathcal{C}(\mathbf{z}_1;\gamma_1)|^{1/2+s/r}m^{-s/r} = c_{r,s}\left(\frac{|\mathcal{C}(\mathbf{z}_1;\gamma_1)|}{|\Omega|}\right)^{1/2+s/r}|\Omega|^{1/2+s/r}m^{-s/r}. \tag{6.2}$$

The constant $c_{r,s}$ depends on r and s, but not on $\mathbf{z}_1$, γ_1, Ω, Q_m, and m.

If $\mathcal{C}(\mathbf{z}_1; \gamma_1)$ covers most of the area of Ω, then the estimate (6.2) is comparable to the estimate (3.1) from Theorem 1 for the case of numerical integration over a spherical cap.

For deriving an upper bound on the worst-case error, we use a spherical cap $\mathcal{C}(\mathbf{z}_2; \gamma_2)$ such that $\Omega \subset \mathcal{C}(\mathbf{z}_2; \gamma_2)$ and obtain the result below, whose proof is sketched at the end of this section.

Theorem 10. *Let $r \geq 2$ and $s > r/2$. Let Ω be a non-empty closed and connected measurable subset of $\mathbb{S}^r$ that is the closure of an open set. Consider a sequence $\{Q_{m(n)}\}_{n\in\mathbb{N}}$ of rules $Q_{m(n)}$ for numerical integration over Ω with the following properties:*

(i) *$Q_{m(n)}$ is of the form (6.1) with $m = m(n)$ nodes located in Ω.*
(ii) *The rule $Q_{m(n)}$ is exact for all spherical polynomials of degree $\leq n$, that is,*

$$Q_{m(n)}[p] = I_\Omega[p] \quad \text{for all } p \in \mathbb{P}_n(\mathbb{S}^r).$$

(iii) *There exist $\mathbf{z}_2 \in \mathbb{S}^r$, $\gamma_2 \in (0, \pi]$, and a positive constant C such that $\Omega \subset \mathcal{C}(\mathbf{z}_2; \gamma_2)$ and such that, for every $Q_{m(n)}$, the weights w_j and nodes $\mathbf{x}_j$ of $Q_{m(n)}$ satisfy the* regularity condition

$$\sum_{\substack{j=1,\\ \mathbf{x}_j \in \mathcal{C}(\mathbf{y};\gamma_2/(\pi n))}}^{m(n)} |w_j| \leq C \left(\frac{\gamma_2}{\pi n}\right)^r \quad \text{for all } \mathbf{y} \in \mathbb{S}^r. \tag{6.3}$$

Then the worst-case error of $Q_{m(n)}$ in $H^s(\mathbb{S}^r)$ satisfies the estimate

$$\begin{aligned} E\big(Q_{m(n)}; H^s(\mathbb{S}^r)\big) &\leq \tilde{c}_{r,s} |\mathcal{C}(\mathbf{z}_2; \gamma_2)|^{1/2+((r+1)/2-\lfloor (r+1)/2\rfloor -1)/(2r)} n^{-s} \\ &= \tilde{c}_{r,s} \left(\frac{|\mathcal{C}(\mathbf{z}_2; \gamma_2)|}{|\Omega|}\right)^{1/2+((r+1)/2-\lfloor (r+1)/2\rfloor -1)/(2r)} |\Omega|^{1/2+((r+1)/2-\lfloor (r+1)/2\rfloor -1)/(2r)} n^{-s}. \end{aligned} \tag{6.4}$$

The positive constant $\tilde{c}_{r,s}$ depends on r, s, and the constant C in (6.3), but not on $\mathbf{z}_2$, γ_2, Ω, $Q_{m(n)}$, $m = m(n)$, and n.

If $\mathcal{C}(\mathbf{z}_2; \gamma_2)$ does not have a much larger area than Ω, then the estimate (6.4) is comparable to the estimate in Theorem 2. A drawback of Theorem 10 seems to be that the regularity condition (6.3) involves the cap $\mathcal{C}(\mathbf{z}_2; \gamma_2)$. However, for any *positive weight* rule $Q_{m(n)}$ that satisfies assumptions (i) and (ii) in Theorem 10, assumption (iii) is automatically satisfied for any spherical cap $\mathcal{C}(\mathbf{z}_2; \gamma_2)$ with $\Omega \subset \mathcal{C}(\mathbf{z}_2; \gamma_2)$ with a constant C that is independent of the rule $Q_{m(n)}$ and the cap $\mathcal{C}(\mathbf{z}_2; \gamma_2)$. This surprising fact follows from the theorem below whose proof follows straight-forwardly by making some slight modifications to the proof of [13, Theorem 6.1].

Theorem 11. *Let $r \geq 2$, and let Ω be a non-empty closed and connected measurable subset of $\mathbb{S}^r$ that is the closure of an open set. Let $\mathcal{C}(\mathbf{z}; \gamma)$, with $\gamma \in (0, \pi]$, be such that $\Omega \subset \mathcal{C}(\mathbf{z}; \gamma)$. Let Q_m, given by (6.1), be any rule for numerical integration over Ω that has nodes $\mathbf{x}_j \in \Omega$, positive weights w_j, and is exact on $\mathbb{P}_n(\mathbb{S}^r)$, where $n \geq 2$. Then*

$$\sum_{\substack{j=1,\\ \mathbf{x}_j \in \mathcal{C}(\mathbf{y};\gamma/(\pi n))}}^{m} w_j = \sum_{\substack{j=1,\\ \mathbf{x}_j \in \mathcal{C}(\mathbf{y};\gamma/(\pi n))}}^{m} |w_j| \leq C \left(\frac{\gamma}{\pi n}\right)^r \quad \text{for all } \mathbf{y} \in \mathbb{S}^r, \tag{6.5}$$

where the positive constant C depends on r, but not on $\mathbf{z}$, γ, Ω, n, m, $\mathbf{y}$ and the rule Q_m.

It should be noted that the constant C in (6.5) is *universal* for all sets $\Omega \subset \mathbb{S}^r$ with the properties stated in Theorem 11, for all spherical caps $\mathcal{C}(\mathbf{z}; \gamma)$ with $\Omega \subset \mathcal{C}(\mathbf{z}; \gamma)$, and for all rules Q_m with the properties stated in Theorem 11.

With Theorem 11 we obtain (as indicated before) the following corollary of Theorem 10.

Corollary 12. *Let $r \geq 2$ and $s > r/2$. Let Ω be a non-empty closed and connected measurable subset of $\mathbb{S}^r$ that is the closure of an open set. Let $\mathbf{z}_2 \in \mathbb{S}^r$ and $\gamma_2 \in (0, \pi]$ be such that $\Omega \subset \mathcal{C}(\mathbf{z}_2; \gamma_2)$. Then there exists a positive constant $\tilde{c}_{r,s}$ (depending only on r and s) such that for every rule $Q_{m(n)}$ for numerical integration over Ω, given by (6.1), that has $m(n)$ nodes in Ω and positive weights and is exact on $\mathbb{P}_n(\mathbb{S}^r)$, where $n \geq 2$,*

$$E\big(Q_{m(n)}; H^s(\mathbb{S}^r)\big) \leq \tilde{c}_{r,s} \left(\frac{|\mathcal{C}(\mathbf{z}_2; \gamma_2)|}{|\Omega|} \right)^{1/2+((r+1)/2-\lfloor (r+1)/2 \rfloor -1)/(2r)} \times |\Omega|^{1/2+((r+1)/2-\lfloor (r+1)/2 \rfloor -1)/(2r)} n^{-s}.$$

It should be noted that the constant $\tilde{c}_{r,s}$ in Corollary 12 is *universal* for all sets $\Omega \subset \mathbb{S}^r$ with the stated properties, for all spherical caps $\mathcal{C}(\mathbf{z}_2; \gamma_2)$ with $\Omega \subset \mathcal{C}(\mathbf{z}_2; \gamma_2)$, and for all rules $Q_{m(n)}$ satisfying the assumptions in Corollary 12.

For proving Theorem 10, the proof of Theorem 2 is modified in the following way: Up to formula (5.19) the proof proceeds exactly as before, where $\mathcal{C}(\mathbf{z}; \gamma)$ has, of course, to be replaced by Ω. Since the integrands in (5.19), with $\mathcal{C}(\mathbf{z}; \gamma)$ replaced by Ω, are non-negative, we obtain an upper bound by increasing the domain of integration in the integrals from Ω to the spherical cap $\mathcal{C}(\mathbf{z}_2; \gamma_2)$ (which contains Ω). This yields the upper bound in (5.19) with $\mathcal{C}(\mathbf{z}; \gamma)$ replaced by $\mathcal{C}(\mathbf{z}_2; \gamma_2)$. Then we need to prove a lemma (for numerical integration over Ω) that is analogous to Lemma 8. After that the proof proceeds as before, where from now on $\mathbf{z}$, γ, and $\mathcal{C}(\mathbf{z}; \gamma)$ need to be replaced by $\mathbf{z}_2$, γ_2, and $\mathcal{C}(\mathbf{z}_2; \gamma_2)$, respectively.

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